7. BIOTIC ALGORITHMS

In this section algorithms for transfers between a biotic compartment type and another biotic or abiotic compartment type are presented. Algorithms are based on diffusive or advective transfer, and most common instances of the latter are transfers via the wildlife diet. Most algorithms apply to all air pollutants, though some that involve octanol-water partition coefficients are only applicable to organic chemicals and mercury species. Some of the equations represent dynamic processes, and others are simple models for which a time-to-equilibrium is calculated. The text box on the next page and continued on the following pages provides a quick summary of the algorithms developed in this chapter and provides a definition of all parameters used. The derivation of chemical-specific algorithms and input parameters is presented in Appendix A.

7.1 SELECTING THE BIOTIC COMPONENTS OF TRIM.FATE

The methodology for determining biotic compartment types is described in Section 3.3 of Volume I of the Technical Support Document for TRIM.FaTE. All major trophic levels in terrestrial and aquatic systems are represented. Default, representative species are chosen based on their prevalence at the test location and/or the availability of parameters for them. Additional species may be chosen based on policy considerations, such as the Endangered Species Act.

General algorithms for plants (Section 7.2.1), soil detritivores (Section 7.2.2), terrestrial mammals and birds (Section 7.2.3) and aquatic biota (Section 7.3) are listed below.

7.2 ALGORITHMS FOR TERRESTRIAL AND SEMI-AQUATIC BIOTA

7.2.1 PLANTS

The plant consists of four compartment types: leaf, stem, root, and the leaf surface (particulate on leaf Lp). Although the leaf surface is not in the plant, it is useful to track because: (1) it is a reservoir of chemical moving to leaves and (2) wildlife diets include particulate matter on leaves.

Several problems arise in modeling uptake and emissions of chemicals by plants.

- Little information is available on the transformations of chemicals within plants.
- The volatilization of chemicals from soils and uptake by plant foliage occurs at a scale that is not easy to model in TRIM.FaTE.
- Little is known about the rate at which chemicals enter plant leaves from particulate matter or rain water on the leaf surface.
- The transport of many chemical species within the plant is not well understood.

Summary of Transport Algorithms Developed in this Chapter

PLANTS

Particulate phase of air to surface of plant leaf (when no rain):

$$T_{Ap \rightarrow Lp} = \frac{v_d I_d A_S}{V_A}$$

Surface of plant leaf to particulate phase of air (when no rain):

$$T_{Lp \rightarrow Ap} = \frac{v_d I_d A_S}{V_A}$$

Vapor phase of air to the leaf surface (during rain):

$$T_{A \rightarrow Lp} = \frac{1}{V_A} \times w_r \times J_{rain} \times A_S \times I_W$$

Particles in air to the leaf surface (during rain):

$$T_{Ap \rightarrow Lp} = \frac{1}{V_A} \times w_r \times J_{rain} \times A_S \times I_W$$

Surface of leaf to surface soil (during rain):

$$T_{LP \rightarrow Ss} = 57.6$$

Leaf surface to leaf:

$$T_{Lp \rightarrow L} = k_{Lp-L}$$

Leaf to leaf surface:

$$T_{L \rightarrow Lp} = 0.01 \times k_{Lp-L}$$

Summary of Transport Algorithms Developed in this Chapter (cont.)

PLANTS (cont.)

Leaf to air (diffusion):

$$T_{L\rightarrow A}^{diff} = (2LAI \times A_S \times g_C + A_S \times g_S) \times \frac{1}{V_L} \times \frac{Z_A}{Z_L}$$

Air to leaf (diffusion):

$$T_{A\rightarrow L}^{diff} = (2LAI \times A_S \times g_C + LAI \times A_S \times g_S) \times \frac{1}{V_A}$$

$$T_{Sr\rightarrow R} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times \frac{\rho area_R}{\rho vol_R} \times \frac{K_{R-Sr}}{d_{Sr}}$$

Root-zone soil to root:
Root to root-zone soil:

$$T_{r\rightarrow Sr} = -\left[\frac{-\ln(1-0.95)}{t_{0.95}}\right]$$

Root-zone soil to stem:

$$T_{Sr\rightarrow St} = \frac{Q_{Xy} \times Z_{water}}{Z_{Sr} \times V_{Sr}} \times TSCF$$

Leaf to stem:

$$T_{L\rightarrow St} = Q_P \times \frac{1}{V_L \times K_{Lp-h}}$$

Stem to leaf:

$$T_{St\rightarrow L} = Q_{Xy} \times \frac{1}{V_{St} K_{St-Xy}}$$

Summary of Transport Algorithms Developed in this Chapter (cont.)

PLANTS (cont.)

Leaf to surface soil (litterfall):

$$T_{L \rightarrow Ss} = L$$

Leaf surface (particulate matter) to surface soil (litterfall):

$$T_{Lp \rightarrow Ss} = L$$

where:

V_A = volume of air volume element (m^3)
v_d = dry deposition velocity of particles (m/d)
I_d = fraction of dry-depositing chemical that is intercepted by plant canopy
A_S = soil area (m^2)
J_{rain} = rain rate (m/d)
w_r = washout ratio (mass chemical/volume rain ÷ mass chemical/volume air)
I_W = interception fraction for wet deposition (unitless)
$k_{Lp\text{-}L}$ = first-order rate constant for transfer of chemical from particles on leaf surface to leaf
LAI = 1-sided leaf-area index (m^2 total leaf area / m^2 underlying soil area)
V_L = volume of leaves (m^3)
Z_P = fugacity capacity (Z-factor) of chemicals in plant (mol-$Pa^{-1}m^{-3}$)
Z_L = fugacity capacity (Z-factor) of chemicals in leaf (mol-$Pa^{-1}m^{-3}$)
g_S = conductance of stomatal pathway, including mesophyll (m/d)
g_C = total conductance of the cuticular path, including the air boundary layer (m/d)
Z_A = fugacity capacity of chemicals in the vapor phase of air (mol$Pa^{-1}m^3$)
$K_{R\text{-}Sr}$ = root-soil partition coefficient (wet kg/kg per wet kg/kg)
$\rho area_R$ = areal density of root in root-zone soil (kg root fresh wt/m^2)
ρvol_R = wet density of root (kg/m^3)
d_{Sr} = depth of root-zone soil (m)
Q_{xy} = flow of transpired water in cell area (m^3/d, below)
$TSCF$ = transpiration stream concentration factor (mg/m^3 of xylem per mg/m^3 of soil pore water)
V_{SrW} = volume of water in root-zone soil (m^3)
Z_{water} = fugacity capacity (Z-value) for water
Z_{Sr} = fugacity capacity (Z-value) for root-zone soil
V_{Sr} = volume of root-zone soil volume element (m^3)
Q_P = phloem flux into fruit (m^3/d), due to advection (assume 5 percent of Q_{xy}, Paterson et al. 1991)
$K_{Lp\text{-}h}$ = partition coefficient between leaves and phloem water (mass/vol to mass/vol)
Q_{xy} = flow of transpired water (m^3/d)
V_{St} = volume of stem (m^3)
$K_{St\text{-}Xy}$ = partition coefficient between stem and xylem water (mass/vol to mass/vol)
L = litterfall rate (d^{-1})

Summary of Transport Algorithms Developed in this Chapter (cont.)

SOIL DETRITIVORES

Root-zone soil to earthworm:

$$T_{Sr\rightarrow worm} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times \frac{\rho area_{worm}}{\rho vol_{worm}} K_{worm-Sr} \frac{1}{d_{Sr}}$$

Earthworm to root-zone soil:

$$T_{worm\rightarrow Sr} = -\left[\frac{-\ln(1-0.95)}{t_{0.95}}\right]$$

Root-zone soil to soil arthropod:

$$T_{Sr\rightarrow arth} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times \rho area_{arth} \times A_S \times \frac{K_{arth-Sr}}{M_{Sr}}$$

Soil arthropod to root-zone soil:

$$T_{arth\rightarrow Sr} = -\left[\frac{-\ln(1-0.95)}{t_{0.95}}\right]$$

where:

$\rho area_{worm}$	=	areal density of earthworm community in root-zone soil (kg worm fresh wt/m^2)
ρvol_{worm}	=	wet density of earthworm (kg/m^3)
$K_{worm-Sr}$	=	earthworm-soil partition coefficient (wet kg/kg per wet kg/kg)
d_{Sr}	=	depth of root-zone soil (v_{sr}/A_S)
A_S	=	soil area (m^2)
$K_{arth-Sr}$	=	arthropod-soil partition coefficient (wet kg/kg per wet kg/kg)
M_{Sr}	=	total mass of root zone soil which contains arthropods (kg)
$\rho area_{arth}$	=	areal density of arthropod community in root-zone soil (kg arthropod fresh wt/m^2)

Summary of Transport Algorithms Developed in this Chapter (cont.)

TERRESTRIAL WILDLIFE

Water to terrestrial vertebrate:

$$T_{w\rightarrow wl} = \rho area_{wl} \times A_S \times \frac{I_w \times A_w}{V_w}$$

Surface soil to terrestrial vertebrate:

$$T_{SS\rightarrow wl} = \rho area_{wl} \times A_S \times \frac{I_{SS} \times A_{SS}}{V_{SS} \times \rho vol_{SS} wet}$$

Plant leaf to terrestrial vertebrate:

$$T_{L\rightarrow wl} = \rho area_{wl} \times \frac{p_P \times I_D \times A_P}{\rho area_L}$$

Surface of plant leaf to terrestrial vertebrate:

$$T_{LP\rightarrow wl} = \rho area_{wl} \times \frac{p_P \times I_D \times A_P}{\rho area_L}$$

Earthworm to terrestrial vertebrate:

$$T_{worm\rightarrow wl} = \rho area_{wl} \times \frac{p_{worm} \times I_D \times A_{worm}}{\rho area_{worm}}$$

Soil arthropod to terrestrial vertebrate:

$$T_{arth\rightarrow wl} = \rho area_{wl} \times \frac{p_{arth} \times I_D \times A_{arth}}{\rho area_{arth}}$$

Terrestrial vertebrate to terrestrial vertebrate:

$$T_{wl\rightarrow wl} = \rho area_{wl} \times \frac{p_{wl} \times I_D \times A_{wl}}{\rho area_{wl}}$$

Summary of Transport Algorithms Developed in this Chapter (cont.)

TERRESTRIAL WILDLIFE (cont.)

Fish to terrestrial vertebrate:

$$T_{f\rightarrow wl} = \rho area_{wl} \times A_S \times \frac{p_f \times I_D \times A_f}{A_{sw} \times \rho area_f}$$

Benthic invertebrate or flying insect to terrestrial vertebrate:

$$T_{bi\rightarrow wl} = \rho area_{wl} \times A_S \times \frac{p_{BI} \times I_D \times A_{BI}}{A_{sw} \times \rho area_{BI}}$$

Air to terrestrial vertebrate:

$$T_{A\rightarrow wl} = \rho area_{wl} \times A_S \times \frac{I_A \times A_A}{V_A}$$

Terrestrial vertebrate to surface soil:

$$T_{wl\rightarrow SS} = f_{uss} E_u$$

Terrestrial vertebrate to water:

$$T_{wl\rightarrow w} = f_{uw} E_u$$

where:

$\rho area_{wl}$	=	wet wildlife biomass density per unit area (kg/m^3, may be calculated as number of animals times average body weight)
A_S	=	area of surface soil (m^2)
I_w	=	water ingestion rate (m^3/kg body weight/d)
V_w	=	volume of water (m^3)
A_w	=	assimilation efficiency of chemical from water (unitless)
I_{SS}	=	surface soil ingestion rate (kg/kg body weight/d)
V_{SS}	=	volume of surface soil (kg)
$\rho vol_{SS}wet$	=	wet bulk density of soil (kg/m^3)
A_{SS}	=	assimilation efficiency of chemical from surface soil (unitless)
p_P	=	proportion of plant matter in diet (unitless)
I_D	=	dietary ingestion rate (kg/kg body weight/d)
A_P	=	assimilation efficiency of chemical from plant in diet (unitless)
$\rho area_L$	=	areal biomass density of foliage (kg/m^2, wet weight)
p_{worm}	=	proportion of earthworm in diet (unitless)
A_{worm}	=	assimilation efficiency of chemical from earthworm in diet (unitless)
$\rho area_{worm}$	=	areal biomass density of earthworms (kg/m^2, wet weight)

Summary of Transport Algorithms Developed in this Chapter (cont.)

TERRESTRIAL WILDLIFE (cont.)

p_{arth}	=	proportion of soil arthropods in diet (unitless)
A_{arth}	=	assimilation efficiency of chemical from soil arthropods in diet (unitless)
p_{wl}	=	proportion of terrestrial wildlife in diet (unitless)
A_{wl}	=	assimilation efficiency of chemical from other wildlife in diet (unitless)
p_f	=	proportion of fish in diet (unitless)
A_f	=	assimilation efficiency of chemical from fish in diet (unitless)
$\rho area_f$	=	areal biomass density of fish (kg/m^2, wet weight, use correct size range for diet)
p_{bi}	=	proportion of benthic invertebrates or emergent flying insects in diet (unitless)
A_{bi}	=	assimilation efficiency of chemical from benthic invertebrates or flying insects in diet (unitless)
A_{sw}	=	area of surface of surface water body (m^2)
$\rho area_{bi}$	=	areal biomass density of benthic invertebrates (kg/m^2, wet weight)
I_A	=	inhalation rate (m^3/kg body weight/d)
V_A	=	volume of air (m^3)
A_A	=	assimilation efficiency of chemical from air (unitless)
E_u	=	chemical elimination through excretory processes (urine and feces) (d^{-1})
f_{uw}	=	fraction of urine and feces excreted to water
f_{uss}	=	fraction of urine and feces excreted to surface soil

AQUATIC BIOTA

Water to macrophytes:

$$T_{w\rightarrow mp} = \frac{V_{mp}\, k_{mp,acc-sw}}{V_w}$$

Macrophytes to water:

$$T_{bi\rightarrow mp} = k_{mp,dep-sw}$$

Water (interstitial or overlying) to benthic invertebrates:

$$T_{w\rightarrow bi} = \frac{n_{bi}\, m_{bi}\, k_{bi,acc-w}}{V_w}$$

Benthic invertebrates to water (interstitial or overlying):

$$T_{bi\rightarrow w} = k_{bi,dep-w}$$

Summary of Transport Algorithms Developed in this Chapter (cont.)

AQUATIC BIOTA (cont.)

Sediment to benthic invertebrates:

$$T_{sed \rightarrow bi} = \frac{n_{bi}\, m_{bi}\, k_{bi,acc-sed}}{V_{sed}\, \rho_{sed}}$$

Benthic invertebrates to sediment:

$$T_{bi \rightarrow sed} = k_{bi,dep-sed}$$

Water to a specific fish domain (*i.e.*, herbivore, omnivore, or carnivore), using the bioenergetic-based kinetic model for nonionic organic chemicals:

$$T_{water \rightarrow fish} = \frac{n_f\, m_f\, k_u}{V_w}$$

A specific fish domain (*i.e.*, herbivore, omnivore, or carnivore) to water, using the bioenergetic-based kinetic model for nonionic organic chemicals:

$$T_{fish \rightarrow water} = k_{eg}$$

A specific fish domain (*i.e.*, benthic omnivore, benthic carnivore, water column herbivore, water column omnivore, or water column carnivore) to the water domain,using the bioenergetic-based kinetic model for mercury:

$$T_{receptor\,(fish) \rightarrow water} = K_E$$

Dietary items to a specific fish domain (*i.e.*, benthic omnivore, benthic carnivore, water column herbivore, water column omnivore, or water column carnivore), using the bioenergetic-based kinetic model:

$$T_{diet \rightarrow receptor\,(fish)} = \frac{n_{receptor}\, m_{receptor}}{n_{diet}\, m_{diet}} \times F_d \times E$$

Dietary items to a specific fish domain (*i.e.*, benthic omnivore, benthic carnivore, water column herbivore, water column omnivore, or water column carnivore), using the time to steady-state-based kinetic model :

$$T_{diet \rightarrow receptor\,(fish)} = \frac{n_{receptor}\, m_{receptor}}{n_{diet}\, m_{diet}} \times \left[\frac{-\ln(1-\alpha)}{t_\alpha} \right] \times K_{receptor-diet}$$

Summary of Transport Algorithms Developed in this Chapter (cont.)

AQUATIC BIOTA (cont.)

A specific fish domain (*i.e.*, benthic omnivore, benthic carnivore, water column herbivore, water column omnivore, or water column carnivore) to the associated dietary items, using the time to steady-state-based kinetic model:

$$T_{receptor\,(fish)\rightarrow diet} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}}\right]$$

where:

$K_{receptor\text{-}diet}$	=	receptor-diet partition coefficient
$k_{mp,acc\text{-}sw}$	=	accumulation from surface water, for macrophytes (1/day)
$k_{mp,dep\text{-}sw}$	=	depuration to surface water, for macrophytes (1/day)
$k_{bi,acc\text{-}sed}$	=	accumulation from sediment, for benthic infauna (1/day)
$k_{bi,acc\text{-}w}$	=	accumulation from water, for benthic infauna (1/day)
$k_{bi,dep\text{-}sed}$	=	depuration to sediment, for benthic infauna (1/day)
$k_{bi,dep\text{-}w}$	=	depuration to water, for benthic infauna (1/day)
k_{eg}	=	elimination via the gills, for fish (1/day)
k_{u}	=	uptake rate constant for fish from water via the gills (1/kg-day)
n_{bi}	=	number of organisms comprising the benthic invertebrate domain
n_{diet}	=	number of contaminated items comprising the potential diet
n_{f}	=	number of organisms comprising a specific fish domain
$n_{receptor}$	=	number of receptors
m_{bi}	=	mass of individual organisms comprising the benthic invertebrate domain (µg)
m_{diet}	=	mass of individual items comprising the potential diet (µg)
m_{f}	=	mass of individual organisms comprising a specific fish domain (µg)
$m_{receptor}$	=	mass of individual receptors (µg)
t_{α}	=	time required to reach α percent of the steady-state value when the concentration in the source is approximately constant with time (day)
V_{mp}	=	volume of the macrophyte in the cell (L)
V_{sed}	=	volume of sediment in the cell (L)
V_{w}	=	volume of water in the cell (L)
ρ_{sed}	=	bulk density of sediment (g/L)
F_{d}	=	feeding rate constant (kg[prey]/kg[predator]-day)
E	=	efficiency of transfer of chemical

- The accumulation of chemicals by wood is not well understood; therefore, trees in TRIM.FaTE consist of leaves only and not stems or roots, except to the extent that stems are conduits of chemicals from leaves.

7.2.1.1 Transfer of Particles and Rain to Surface of Leaf

The surface of the leaf includes: dry particulate matter deposited to the plant surface, particles deposited to the plant surface in rain water, and rain water containing gaseous chemical. Deposition is defined here as the mass transfer of suspended particulates from air to the plant surface. Elsewhere (*e.g.*, Lindberg et al. 1992), the deposition of chemicals to plants is defined to include the gaseous fraction of the pollutants that come into contact with plants. The uptake of gaseous pollutants in TRIM.FaTE is treated below.

Dry or wet deposition to the surface of the leaf is the deposition velocity times the leaf interception fraction. The leaf interception fraction (I) is the fraction of particles that land on the leaf; thus 1-I is the fraction that lands on soil. It is common for a concentration of a deposited particulate chemical to be estimated with respect to the leaf or above-ground plant mass. However, when that concentration is estimated, it is often forgotten that most of the chemical mass is still *on* the plant rather than *in* it.

Dry Deposition of Particles to Surface of Plant Leaves

Dry deposition is estimated by multiplying the predicted air concentration at ground level by the deposition velocity (U.S. EPA 1997a). Thus, a flux equation that expresses dry deposition to the leaf, from van de Water (1995) follows. Note that the area of soil and that associated with an air volume element may be different.

$$\frac{dN_{Lp}}{dt} = \frac{N_{Ap}}{V_A} v_d I_d A_S \qquad (7\text{-}1)$$

where:

N_{Lp} = mass of chemical depositing on leaf surfaces from particulate matter in air (kg)
N_{Ap} = mass of particle-bound chemical in air (kg)
V_A = volume of air volume element (m^3)
v_d = dry deposition velocity of particles (m/d)
I_d = fraction of dry-depositing chemical that is intercepted by plant canopy (unitless, below)
A_S = soil area (m^2)

The interception fraction for dry deposition (I_d) may be calculated using the following equation (Baes et al. 1984):

$$I_d = 1 - e^{(1-W_L)(-\alpha \times \rho area)} \quad (7\text{-}2)$$

where:

α = vegetation attenuation factor (m^2/kg)
$\rho area$ = wet above-ground non-woody vegetation biomass inventory per unit area (kg/m^2)
W_L = water content of leaf (mass/mass, unitless)

The water content adjusts ρarea to represent dry biomass. The equation was originally derived for pasture grasses and hay and expanded to other crops. For this reason, the biomass should not include wood. The vegetation attenuation factor (sometimes called the foliar interception constant) is sometimes equivalent to the surface area of leaves divided by plant biomass (van de Water 1995) or the leaf biomass if the plant is woody.

Thus,

$$T_{Ap \rightarrow Lp} = \frac{v_d I_d A_S}{V_A} \quad (7\text{-}3)$$

where:

$T_{Ap\text{-}Lp}$ = transfer factor from particulate phase of air to surface of plant leaf (process occurs when it is not raining)

If it is assumed that particles are blown off the plant with wind at a rate that equals the deposition rate to leaves, and all particles are dispersed in air,

$$T_{Lp \rightarrow Ap} = \frac{v_d I_d A_S}{V_A} \quad (7\text{-}4)$$

where:

$T_{Lp \rightarrow Ap}$ = transfer factor from surface of plant leaf to particulate phase of air (process occurs when it is not raining)

Wet Deposition to Plants

Rain scavenges some of the chemical mass from the vapor phase and particulate phase of air. Wet deposition resulting from these processes may be modeled distinctly with the same equation. The rate of mass transfer of vapor-phase or particulate phase mercury from air to rain

water and to the surface of the plant leaf is described by the following equation (modified from van de Water 1995):

$$\frac{dN_{Lp}}{dt} = \frac{N_A}{V_A} \times w_r \times J_{rain} \times A_S \times I_W \quad (7\text{-}5)$$

where:

N_{Lp}	=	mass of chemical on surface of leaf (kg)
N_A	=	mass of chemical in gas phase of air (kg)
V_A	=	volume of air (m^3)
J_{rain}	=	rain rate (m/d)
w_r	=	washout ratio (mass chemical/volume rain ÷ mass chemical/volume air)
A_S	=	area of soil (m^2)
I_W	=	interception fraction for wet deposition (unitless)

The interception fraction may be calculated using the following equation from Muller and Prohl (1993). The fraction is dependent on how much water the leaf can hold, the total amount of rainfall, and the ability of the element or compound to stick to the leaf.

$$I_w = \frac{LAI \times S}{rain}\left[1 - e^{\left(\frac{-\ln 2}{3S} \times rain\right)}\right] \quad (7\text{-}6)$$

where:

LAI	=	1-sided leaf-area index (m^2 total leaf area / m^2 underlying soil area)
S	=	vegetation-dependent leaf-wetting factor (retention coefficient) (m)
$rain$	=	amount of rainfall of a rainfall event (m)

If I_w is calculated to be greater than 1, then the value must be set to 1. Thus,

$$T_{A-Lp} = \frac{1}{V_A} \times w_r \times J_{rain} \times A_S \times I_W \quad (7\text{-}7)$$

where:

$T_{A\text{-}Lp}$	=	the transfer factor from the vapor phase of air to the leaf surface

The rate of mass transfer of particulate-phase mercury from air to rain water and to the surface of the plant leaf may be described by an analogous equation:

$$\frac{dN_{Lp}}{dt} = \frac{N_{Ap}}{V_A} \times w_r \times J_{rain} \times A_S \times I_W \quad (7\text{-}8)$$

where:

N_{Lp} = mass of chemical on surface of leaf (kg)
N_{Ap} = mass of chemical in particulate phase of air (kg/m^3)
V_A = volume of air (m^3)
w_r = washout ratio (mass chemical/volume rain ÷ mass chemical/volume air)
J_{rain} = rate of rainfall (m/d)
A_S = area of soil (m^2)
I_W = interception fraction (unitless, see equation above)

Thus,

$$T_{Ap \rightarrow Lp} = \frac{1}{V_A} \times w_r \times J_{rain} \times A_S \times I_W \tag{7-9}$$

where:

$T_{Ap \rightarrow Lp}$ = the transfer factor from particles in air to the leaf surface

Washoff of Chemical from Plant Surface

It has been observed that particles on the surface of conifer leaves are washed off (during rain events) according to first-order kinetics with a rate constant of 0.04 per min (McCune and Lauver 1986). The rate of 0.04 per min is equivalent to 2.4 per hour or 57.6 per day. It may be assumed that the particles deposited in rain water and the chemical dissolved in rain water is washed off at the same rate. Thus,

$$\frac{dN_{Lp}}{dt} = -57.6 \times N_{Lp} \tag{7-10}$$

and

$$T_{Lp \rightarrow Ss} = 57.6 \tag{7-11}$$

where:

$T_{Lp \rightarrow Ss}$ = transfer factor from surface of leaf to surface soil during rain (d^{-1})

An alternative type of transfer would be an instantaneous transfer at the end of a rain event, where the transfer would also be derived from McCune and Lauver (1986):

$$T_{LP \rightarrow Ss} = 1 - e^{-0.0003 rain} \tag{7-12}$$

where:

$T_{Lp \rightarrow Ss}$ = transfer factor from surface of leaf to surface soil during rain (instantaneous)
rain = cumulative amount of rain during rain event (m)

The implementation of this transfer may be required if the high first-order rate constant above (which is equivalent to 2.4 per hour) causes instability in LSODE, the differential equation solver.

Note that it may not be assumed that the transfer factor for loss to soil is the same as the transfer from the vapor phase of air or particles in air via rain (as is assumed with dry deposition). In order to have this option, the vapor phase and particulate phase of the chemical in rain water on the surface of the leaf would have to be tracked separately, and two transfer factors to surface soil would be required.

Transfer of Chemical to Leaf from Particles on Plant

The fraction of deposited chemical that enters the plant cuticle per day is very uncertain. It depends on the relative concentrations in the plant and particles at equilibrium (which is unknown), as well as the time to equilibrium. It is sometimes assumed that chemicals attached to particles reach instantaneous solution equilibrium with plant tissues when they land on the plant. If that assumption is made for some chemicals (*e.g.*, mercury), TRIM.FaTE is likely to overestimate the contribution of the particles to uptake of the chemical by the plant (Lindberg 1999a). For a chemical that is tightly and chemically bound to particles in air (*e.g.*, Hg), an initial assumption of 0.2 per day may be appropriate. Because particles cover only a small fraction of the surface of the plant, it is assumed that the rate of transfer from leaves to particles is 1 percent of the rate of transfer in the other direction (0.002 per day). The rate may be higher for the transfer of mercury from the plant to a dissolved state in rain water, but no information is available on this. Note that these default values will change if units of time change.

$$T_{Lp \rightarrow L} = k_{LP-L} \tag{7-13}$$

$$T_{L \rightarrow Lp} = 0.01 \times k_{LP-L} \tag{7-14}$$

where:

$T_{Lp \rightarrow L}$ = transfer factor from leaf surface to leaf
$T_{L \rightarrow Lp}$ = transfer factor from leaf to leaf surface

Transformations on the Leaf

Transformations of chemicals in particulate matter on the surface of plant leaves are assumed to occur at the same rate as transformations in air.

7.2.1.2 Uptake of Gaseous Chemical into Foliage

The diffusion pathway is valid for all gaseous forms of chemicals, including organic compounds and mercury species. The diffusion from air to plants is based on two resistances in parallel: a) the series resistance of stomata and mesophyll and b) the series resistance of air and cuticle. It is assumed that a chemical fraction that is in the plant cuticle or mesophyll is inside of the plant, but that the chemical inside of the stoma but outside of the mesophyll is outside of the plant. It should be noted that the resistance is the inverse of the conductance. Damage to the plant (*e.g.*, from insect herbivory) can also contribute significantly to the transport of nutrients from plant leaves (Hargrove 1999). However, the contribution of insect or other sources of damage to the diffusion of Hg into and out of the plant is unknown and not incorporated into TRIM.FaTE.

Stomatal Conductance

The stomatal conductance of gaseous chemicals into the leaf may be determined based on the stomatal conductance of water vapor. The only chemical-specific parameter that is required is the molecular weight of the chemical. One means to estimate the stomatal conductance is the following

$$g_{stomata} = \sqrt{18 / MW} \times g_{water} \tag{7-15}$$

where:

$g_{stomata}$ = conductance of chemical through the stomata (m/s)
g_{water} = conductance of water through the stomata (m/s)
MW = molecular weight of chemical

Conductance of water through the stomata may be calculated using one of the following algorithms. The first is taken from Bennett et al. (1998) and Trapp (1995) and has been implemented in TRIM.FaTE:

$$g_{water} = \frac{461 \times T}{(1 - rh) \times 611 \times 10^{\frac{7.5(T-273)}{(237+(T-273)}}} \times \left(1\,\text{kg} \times \text{d}^{-1} \times \text{m}^2\right) \tag{7-16}$$

where:

g_{water} = conductance through the stomata (m/d)
Z_A = fugacity capacity of chemicals in the vapor phase of air ($\text{molPa}^{-1}\text{m}^3$)
rh = relative humidity (unitless)
T = temperature (degrees Kelvin)

Stomatal conductance of water and chemicals should be adjusted to zero at night.

Alternatively, the stomatal conductance of water may be calculated (Riederer 1995) using the following equation. This option has not yet been implemented in TRIM.FaTE:

$$g_{water} = \frac{D_A^{H_2O} na_S \alpha}{x_S + y_S} \tag{7-17}$$

where:

g_{water}	=	conductance of water through the stomata (m/d)
D_A^{H2O}	=	diffusion coefficient of water in air (m^2/d)
na_S	=	number of stomata in leaf (n) times area of 1 stoma divided by area of leaf (a_S)
α	=	mean degree of opening of stomatal pores, between 0 and 1
x_S	=	depth of elliptical pore (m)
y_S	=	mean pore radius (m)

If this latter algorithm is used, it should be noted that conductance varies with temperature. In the 20° to 40°C temperature range, the vapor flux from leaves has been observed to double with a 10° rise in temperature (Leonard et al. 1998), so variability in temperature could contribute significantly to the uncertainty in this type of transfer.

Mesophyll Conductance

It is suggested that for most organic chemical species and most plant species, the stomatal or cuticular conductance is the rate-limiting pathway (Riederer 1995). Therefore, for most chemicals, there is no need to consider mesophyll (inner tissue) conductance. However, some work with mercury cited in Lindberg et al. (1992) suggests that "resistance on or within mesophyll surfaces dominates the atmosphere-leaf diffusive path of Hg^0." See Section A.1.1 of Appendix A.

Total Conductance of the Stomatal Pathway

Thus, the total conductance of the stomatal pathway is:

$$g_S = \left(\frac{1}{g_{Stomata}} + \frac{1}{g_m} \right)^{-1} \tag{7-18}$$

where:

g_S	=	conductance of stomatal pathway, including mesophyll (m/d)
$g_{Stomata}$	=	conductance of stomata (m/d)
$g_{Stomata}$	=	conductance of mesophyll (m/d)

Boundary-layer Conductance

The boundary-layer conductance is defined by the following equation:

$$g_B = \frac{D_A}{\delta_{AP}} \tag{7-19}$$

where:

g_B = conductance of the boundary layer (m/d)
D_A = diffusion coefficient of chemical through still air (m^2/d)
δ_{AP} = thickness of air boundary layer over plant (m)

The boundary layer thickness (δ_{AP} in m) may be approximated by the following equation (Nobel 1991), or the value may be assumed (*e.g.*, 0.001 m in Riederer 1995, 0.005 m in McKone 1993a,b,c). The constant of 0.004 is the square root of the viscosity of air at 20 degrees Celsius, 1.51 x 10^{-5} m^2 per second (Wilmer and Fricker 1996).

$$\delta_{AP} = 0.004\sqrt{l/v} \tag{7-20}$$

where:

l = length of flat leaf (m)
v = wind velocity (m/s)

Cuticular Conductance

The cuticular conductance (mass transfer coefficient from air outside of the plant to the cuticle) is defined by the following equation (Riederer 1995):

$$g_{cuticle} = \frac{P_C}{K_{AW}} \tag{7-21}$$

where:

$g_{cuticle}$ = conductance of the cuticle (m/s)
P_C = permeance of the cuticle (m/s)
K_{AW} = air-water partition coefficient (unitless)

Cuticular permeance has been measured in *Citrus aurantium* leaves, and the following relationship was derived (Riederer 1995). The variability of this relationship with plant species is unknown.

$$\log P_c = 0.704 \log K_{ow} - 11..2 \quad (r = 0.91) \tag{7-22}$$

In addition, K_{AW} is equivalent to Z_{Air}/Z_W. Thus,

$$g_{cuticle} = \left(\frac{10^{0.704 \log K_{ow} - 11.2}}{Z_{AIR} / Z_w} \right) \times 24 \times 60 \times 60 \quad (7\text{-}23)$$

where:

$g_{cuticle}$ = conductance of the cuticle (m/d, note change in units)
Z_W = capacity (Z-factor) of chemicals in water ($molPa^{-1}m^3$)
Z_{air} = capacity (Z-factor) of chemicals in air, including particulates ($molPa^{-1}m^3$)

The cuticular conductance must be put in series with resistance through the air on the leaf surface to yield the total cuticular conductance (air to plant), adjusted for capacity (Z-factor) of the air and leaf. Thus:

$$g_C = \left(\frac{1}{g_B} + \frac{1}{g_{cuticle}} \right)^{-1} \quad (7\text{-}24)$$

where:

g_B = conductance of the boundary layer (m/d)
$g_{cuticle}$ = conductance of the cuticle (m/d)
g_C = total conductance of the cuticular path, including the air boundary layer (m/d)

Riederer (1995) has derived the flux equation for diffusion in and out of plant leaves.

$$\frac{dN_L}{dt} = A(g_C + g_S)\frac{N_A}{V_A} - A(g_C + g_S)\frac{N_L}{V_L} \times \frac{K_{AW}}{K_{LW}} \quad (7\text{-}25)$$

where:

N_L = mass of chemical in leaf compartment (g)
N_A = mass of chemical in air compartment (g)
V_A = volume of air compartment (m^3)
V_A = volume of leaf compartment (m^3)
K_{LW} = air/leaf partition coefficient (unitless)

Transfer Factors for Diffusion

If the Bennett et al. (1998) equation (which is calculated with respect to soil area) is used for the stomatal conductance, the transfer factor for diffusion from leaf to air is:

$$T_{L-A}^{diff} = (2LAI \times A_S \times g_C + A_S \times g_S) \times \frac{1}{V_L} \times \frac{Z_A}{Z_L} \quad (7\text{-}26)$$

where:

V_L	=	volume of leaves (m^3)
LAI	=	Leaf-area index, the area of one side of a leaf (unitless)
A_S	=	area of soil (m^2)
Z_P	=	capacity (Z-factor) of chemicals in plant (mol-$Pa^{-1}m^{-3}$)
Z_L	=	capacity (Z-factor) of chemicals in leaf (mol-$Pa^{-1}m^{-3}$)

Note that the contact area associated with the cuticular pathway is 2 times the LAI (because cuticles cover the top and bottom of a leaf). If the Riederer (1995) equation (which is calculated with respect to 1-sided leaf area) is used for the stomatal conductance, the transfer factor is:

$$T_{L-A}^{diff} = (2LAI \times A_S \times g_C + LAI \times A_S \times g_S) \times \frac{1}{V_L} \times \frac{Z_A}{Z_P} \quad (7\text{-}27)$$

Z_P may be calculated using the following equation, which represents plants as mixture of air, water and nonpolar organic matter analogous to octanol (Paterson and Mackay 1995). It is assumed that the fugacity capacity of a plant leaf is equivalent to that of a generic plant that is 18 percent air, 80 percent water, and 2 percent nonpolar organic matter.

$$Z_P = 0.18\ Z_A + 0.80\ Z_W + 0.02\ K_{OW}\ \text{x}\ Z_W \quad (7\text{-}28)$$

Similarly, if the Bennett et al. (1998) equation (which is calculated with respect to soil area) is used for the stomatal conductance, the transfer factor for diffusion from air to leaf is:

$$T_{A-L}^{diff} = (2LAI \times A_S \times g_C + A_S \times g_S) \times \frac{1}{V_A} \quad (7\text{-}29)$$

And if the Riederer (1995) equation (which is calculated with respect to 1-sided leaf area) is used for the stomatal conductance, the transfer factor is:

$$T_{A-L}^{diff} = (2LAI \times A_S \times g_C + LAI \times A_S \times g_S) \times \frac{1}{V_A} \quad (7\text{-}30)$$

7.2.1.3 Uptake from Soil by Root

The uptake of chemicals by plant roots is treated as an equilibrium process. Two alternative algorithms may be used to calculate the accumulation of a chemical by plants from

soil: uptake from soil or uptake from soil water. Both algorithms are derived from an equilibrium relationship, an estimated time to equilibrium, and the assumption of a first order rate of uptake. These algorithms do not apply to woody tree roots or tuber crops. Uptake of chemicals by these types of roots is not considered in TRIM.FaTE at this time.

Uptake from Whole Soil

The uptake of chemicals by roots in TRIM.FaTE is described by an equation in the form of a time to equilibrium between the roots and soil. Because of the linear relationships in TRIM.FaTE, uptake is described as proportional to the concentration of the chemical in soil even though some studies suggest that a log-log regression between soil and root concentrations is a more precise model of uptake.

$$C_{R-dry} = K_{RSr-dry} \times C_{Sr-dry} \tag{7-31}$$

where:

$C_{R\text{-}dry}$	=	concentration of chemical in dry root (kg/m^3, dry wt)
$K_{RSr\text{-}dry}$	=	dry root/root-zone-soil partition coefficient (uptake factor, dimensionless)
$C_{Sr\text{-}dry}$	=	concentration of chemical in root-zone soil (kg/m^3, dry wt)

If masses are converted to wet mass, then:

$$C_R = (1\text{-}W_R) \times C_{R\text{-}dry} \tag{7-32}$$

where:

W_R	=	water content of root (kg water/kg worm)
C_R	=	total concentration of chemical in root (kg/m^3)

and

$$C_{Sr} = (1\text{-}W_{Sr}) \times C_{Sr\text{-}dry} \tag{7-33}$$

where:

W_{Sr}	=	water content of soil (kg water/kg root zone soil)
C_{Sr}	=	total concentration of chemical in root zone soil (kg/m^3)

Thus,

$$(1-W_R) \times C_{R-dry} = \frac{(1-W_R) \times K_{R-Sr(dry)}}{1-W_{Sr}} \times (1-W_{Sr}) \times C_{Sr-dry} \tag{7-34}$$

and

$$C_R = K_{R-Sr} \times C_{Sr} \tag{7-35}$$

where:

$K_{R\text{-}Sr}$ = root-soil partition coefficient (wet kg/kg per wet kg/kg), calculated to be:

$$K_{R-Sr} = \frac{(1 - W_R) \times K_{R-Sr-dry}}{1 - W_{Sr}} \tag{7-36}$$

Thus,

$$\frac{dC_R}{dt} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times K_{R-Sr} \times C_{Sr} - \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] C_R \tag{7-37}$$

where:

$t_{0.95}$ = time required to reach 95 percent of the steady-state value when C_{Sr} is approximately constant with time (d)

If the areal density of roots is approximately constant with time, then:

$$\frac{dN_R}{dt} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times V_R \times K_{R-Sr} \times \frac{N_{Sr}}{V_{Sr}} - \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] N_R \tag{7-38}$$

where:

N_R = mass of chemical in nonwoody roots (kg)
N_{Sr} = total mass of chemical in all phases of bulk root-zone soil (kg)
V_{Sr} = total volume of root-zone soil, which contains roots (m^3)
V_R = total volume of roots (m^3)

and

$$V_R = \frac{\rho area_R \times A_S}{\rho vol_R} \tag{7-39}$$

where:

A_S = area of soil surface (m^2)
$\rho area_R$ = areal density of root in root-zone soil (kg root fresh wt/m^2)

ρvol_R = wet density of root (kg/m^3)

Transfer Factors

$$T_{Sr-R} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times \frac{\rho area_R}{\rho vol_R} \times \frac{K_{R-Sr}}{d_{Sr}} \tag{7-40}$$

$$T_{r-Sr} = -\left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \tag{7-41}$$

where:

T_{Sr-R} = transfer factor from root-zone soil to root
T_{R-Sr} = transfer factor from root to root-zone soil

Uptake from Soil Water

An alternative method by which to estimate the root concentration of a chemical is an equilibrium between root tissue and soil water concentration. The equilibrium relationship is a generalization of the Briggs et al. (1982) equation developed in Trapp (1995).

$$C_R = K_{R-SrW} \times C_{SrW} \tag{7-42}$$

where:

C_R = concentration in roots (kg [chemical]/m^3 [root fresh weight])
$K_{R\text{-}Sr\,W}$ = root - root zone soil water partition coefficient (kg/m^3 per kg/m^3) (below)
C_{sw} = concentration in soil pore water (kg [chemical]/m^3 [soil pore water])

$$K_{R-SrW} = (W_R + L_R K_{ow}^b)\rho vol_R \rho vol_{SW}^{-1} \tag{7-43}$$

where:

W_R = water content of root (mass/mass wet weight)
L_R = lipid content of root (mass/mass wet weight)
b = correction exponent for the differences between octanol and lipids
ρvol_R = density of fresh root (g [root]/cm^3 [root])
ρvol_{SW} = density of soil pore water (g [soil pore water]/cm^3 [soil pore water])

Thus,

$$\frac{dC_R}{dt} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times K_{R-SrW} \times C_{SrW} - \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] C_R \tag{7-44}$$

where:

$t_{0.95}$ = time required to reach 95 percent of the steady-state value when C_{Sr} is approximately constant with time (d)

If the areal density of roots is approximately constant with time, then:

$$\frac{dN_R}{dt} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times V_R \times K_{R-SrW} \times \frac{N_{SrW}}{V_{SrW}} - \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] N_R \quad (7\text{-}45)$$

where:

N_R = mass of chemical in nonwoody roots (kg)
N_{SrW} = total mass of chemical in root-zone soil water (kg)
V_{SrW} = volume of root-zone soil water (m^3)
V_R = total volume of fresh roots in parcel (m^3)

$$V_R = \frac{\rho area_R \times A_S}{\rho vol_R} \quad (7\text{-}46)$$

where:

A_S = area of soil surface (m^2)
$\rho area_R$ = areal density of root in root-zone soil (kg root fresh wt/m^2)
ρvol_R = wet density of root (kg/m^3)

The transfer factors are:

$$T_{SrW-R} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times \frac{\rho area_R}{\rho vol_R} \times \frac{K_{R-SrW}}{d_{Sr}} \quad (7\text{-}47)$$

$$T_{R-SrW} = -\left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \quad (7\text{-}48)$$

where:

$T_{SrW\text{-}R}$ = transfer factor from root-zone soil water to root
$T_{R\text{-}SrW}$ = transfer factor from root to root-zone soil water

7.2.1.4 Uptake by Stem

The algorithms for the uptake of chemicals by the stem are taken from Trapp (1995) who derived them for organic chemicals.

Contribution from Soil Pore Water via Transpiration Stream (Xylem)

$$\frac{dN_{St}}{dt} = Q_{XY} \times TSCF \times \frac{N_{SrW}}{V_{SrW}} \tag{7-49}$$

where:

N_{St} = mass in all stems in volume element (kg)
Q_{XY} = flow of transpired water in cell area (m^3/d, below)
$TSCF$ = transpiration stream concentration factor (mg/m^3 of xylem per mg/m^3 of soil pore water)
N_{SrW} = mass of chemical in root-zone soil water (kg)
V_{SrW} = volume of water in root-zone soil (m^3)

According to Crank et al. (1981),

$$Q_{Xy} = 4.8 \times 10^{-3} \times LAI \times A_S \tag{7-50}$$

where:

4.8×10^{-3} = empirical factor with units of m/d
LAI = leaf-area index
A_S = area of soil (m^2)

Thus,

$$T_{Sr-St} = \frac{Q_{Xy} \times Z_{water}}{Z_{Sr} \times V_{Sr}} \times TSCF \tag{7-51}$$

where:

$T_{Sr\text{-}St}$ = transfer for root-zone soil to stem

Contribution from Leaves via Phloem

Assuming that the chemical concentration in phloem sap is in equilibrium with that in leaves,

$$\frac{dN_{St}}{dt} = Q_P \times \frac{N_L}{V_L \times K_{LPh}} \quad (7\text{-}52)$$

where:

N_{St} = mass of chemical in stems in volume element (kg)
Q_P = phloem flux into fruit (m^3/d), due to advection (assume 5 percent of Q_{xy}, Paterson et al. 1991)
N_L = mass of chemical in leaves (kg)
V_L = volume of leaves (m^3)
K_{LPh} = partition coefficient between leaves and phloem water (mass/vol to mass/vol)

The following equation, adapted from an equation for sorption of contaminants to plant roots (Trapp 1995), may be used to calculate K_{LPh}.

$$K_{LPh} = (W_L + l_L \times K_{ow}^b) \times \rho vol_L \; / \; \rho vol_{Ph} \quad (7\text{-}53)$$

where:

W_L = water content of leaves (mass/mass wet weight)
l_L = lipid content of leaves (mass/mass wet weight)
b = correction exponent for differences between foliage lipids and octanol
ρvol_L = density of leaf (kg/m^3)
ρvol_{Ph} = density of phloem (kg/m^3)

If the chemical in question is ionic, it may be assumed that K_{ow} is close to zero and that the concentration of the ionic species in phloem is the same as that in leaf water.

Thus,

$$T_{L-St} = Q_P \times \frac{1}{V_L \times K_{LPh}} \quad (7\text{-}54)$$

where:

$T_{L\text{-}St}$ = transfer factor for leaf to stem

Loss with Xylem to Leaves

$$\frac{dN_L}{dt} = Q_{Xy} \times \frac{N_{St}}{V_{St} K_{StXy}} \quad (7\text{-}55)$$

where:

N_L = mass of chemical in leaves (kg)
Q_{xy} = flow of transpired water (equation above)
N_{St} = mass of chemical in stem (kg)
V_{St} = volume of stem (m^3)
K_{StXy} = partition coefficient between stem and xylem water (mass/vol to mass/vol)

The following equation, adapted from an equation for sorption of contaminants to plant roots (Trapp 1995), may be used to calculate K_{StXy}.

$$K_{StXy} = (W_{St} + l_{St} \times K_{ow}^{b}) \times \rho vol_{St} \; / \; \rho vol_{Xy} \quad (7\text{-}56)$$

where:

W_{St} = water content of stem (mass/mass wet weight)
l_{St} = lipid content of stem (mass/mass wet weight)
K_{ow} = octanol-water partition coefficient
b = correction exponent for differences between foliage lipids and octanol
ρvol_{St} = density of stem (mass wet weight/volume)
ρvol_{Xy} = density of xylem fluid (mass wet weight/volume)

If the chemical in question is ionic, it may be assumed that K_{ow} is zero and that the concentration of the ionic species in xylem is the same as that in leaf water.

Thus,

$$T_{St-L} = Q_{Xy} \times \frac{1}{V_{St} K_{StXy}} \quad (7\text{-}57)$$

where:

$T_{St\text{-}L}$ = transfer factor for stem to leaf

Loss from Phloem to Fruit

It is not necessary to implement a fruit compartment or this loss term in TRIM.FaTE unless a) moderate to high concentrations of the chemical have been found in fruit and b) fruit constitutes a significant portion of the biomass of the vegetation. This algorithm has not yet been

implemented in any tests of TRIM.FaTE. The concentration of any chemical in the phloem running through the stem is at the same concentration as xylem sap leaving the stem; both are in equilibrium with the stem. Thus,

$$\frac{dN_{PhF}}{dt} = Q_P \times \frac{N_{St}}{V_{St} K_{StXy}} \tag{7-58}$$

where:

N_{PhF}	=	mass of chemical in fruit (kg)
V_F	=	volume of fruit (m^3)
Q_P	=	phloem flux into fruit (m^3/d), due to advection (assume 5 percent of Q_{xy}, Paterson et al. 1991)
N_{st}	=	mass of chemical in stem (kg)
V_{st}	=	volume of stem (m^3)
K_{StXy}	=	partition coefficient between stem and xylem water (mass/vol to mass/vol)

Stem Simplifications for Nonionic Organic Chemicals

The uptake of nonionic organic chemicals by the stem is assumed to originate from the root. Little if any nonionic organic chemical mass is transported from leaves to stems. For that reason, in the PAH test case of TRIM.FaTE, the root and stem were not connected to the leaves. The algorithm for uptake by the stem was an equilibrium relationship taken from Briggs et al. (1983):

$$C_{stem} = SCF \times C_{SrW} \times \rho vol_{stem} \rho vol_{SrW}^{-1} \tag{7-59}$$

where:

C_{stem}	=	concentration of chemical in stem (kg [chemical]/m^3 [stem])
C_{SrW}	=	concentration in soil water (kg/m^3)
SCF	=	stem concentration factor (kg/kg per kg/kg) (below)
ρvol_{stem}	=	density of stem, kg (fresh stem)/m^3 (fresh stem)
ρvol_{SrW}	=	density of soil water, kg (soil water)/m^3 (soil water)

The stem concentration factor may be calculated by the following equation from Briggs et al. (1983):

$$SCF = (10^{0.95 \log K_{ow} - 2.05} + 0.82) \times 0.784 \times e^{-(\log K_{ow} - 1.78)^2 / 2.44} \tag{7-60}$$

Thus,

$$\frac{dC_{stem}}{dt} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times SCF \times \frac{\rho vol_{stem}}{\rho vol_{SrW}} \times C_{SrW} - \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] C_{stem} \quad (7\text{-}61)$$

where:

$t_{0.95}$ = time required to reach 95 percent of the steady-state value when C_{Sr} is approximately constant with time (d)

If the areal density of stems is approximately constant with time, then:

$$\frac{dN_{stem}}{dt} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times V_{stem} \times SCF \times \frac{\rho vol_{stem}}{\rho vol_{SrW}} \times \frac{N_{SrW}}{V_{SrW}} - \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] N_{stem} \quad (7\text{-}62)$$

where:

N_{stem} = mass of chemical in fresh stems (kg)
N_{SrW} = total mass of chemical in root-zone soil water (kg)
V_{SrW} = volume of root-zone soil water (m^3)
V_{stem} = total volume of fresh stems in parcel (m^3)

$$V_{stem} = \frac{\rho area_{stem} \times A_S}{\rho vol_{stem}} \quad (7\text{-}63)$$

where:

A_S = area of soil surface (m^2)
$\rho area_{stem}$ = areal density of stem in root-zone soil (kg root fresh wt/m^2)
ρvol_{stem} = wet density of stem (kg/m^3)

The transfer factors are:

$$T_{SrW \rightarrow stem} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times \rho area_{stem} \times \frac{SCF}{\rho vol_{SrW} \times d_{Sr}} \quad (7\text{-}64)$$

$$T_{stem \rightarrow SrW} = -\left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \quad (7\text{-}65)$$

where:

$T_{SrW \rightarrow stem}$ = transfer factor from root-zone soil water to stem
$T_{stem \rightarrow SrW}$ = transfer factor from stem to root-zone soil water

7.2.1.5 Uptake by Wood and Tree Bark

Wood is of interest in a mass-balanced chemical transport and fate model because of its potential for serving as a large reservoir of chemical mass. The few studies that exist suggest that there is some accumulation of air pollutants in bark and wood. Ralph Turner (1998) has limited data on the accumulation of mercury in wood, but the mechanism of accumulation is not understood. Simonich and Hites (1995) provide data on the accumulation of organochlorine compounds in tree bark; polycyclic aromatic hydrocarbons would be expected to have similar properties. The transfer of chemicals to wood and tree bark is not modeled because of a general lack of information for persistent air pollutants.

7.2.1.6 Chemical Transformations

All transformations are assumed to be first-order processes in TRIM.FaTE. The derivations of these values for particular chemicals (*e.g.*, PAHs and Hg) are described in Appendix A of this volume.

7.2.1.7 Litterfall

The flux of chemical from leaves to surface soil may be expressed by the equation:

$$\frac{dN_{Ss}}{dt} = L \times N_L + L \times N_{Lp} \quad (7\text{-}66)$$

where:

N_{Ss} = mass of chemical in surface soil in cell (kg)
L = litterfall rate (d^{-1})
N_L = mass of chemical in foliage in cell (kg)
N_{Lp} = mass of chemical on surface of leaves in cell (kg)

It is assumed that all leaves of deciduous trees are dropped to surface soil between the day of first frost and a date that is 30 days later. Thus, $L = 1/30\ d^{-1}$.

Conifers drop their leaves at a steady rate, with a complete turnover which lasts 2 to 10 or 11 years (Post 1999). It is assumed for the purpose of TRIM.FaTE that the leaf turnover is 6 years. Thus, $L = 1/2190\ d^{-1}$.

It is assumed that herbaceous plants and grasses become "litter" on the surface of the soil during the 30 day period beginning the day of first frost. Thus, $L = 1/30\ d^{-1.}$

It is assumed that agricultural plants are harvested and do not become "litter." If agriculture were dominant, this assumption would need to be revised, based on harvesting practices (*e.g.*, how much residue is left) for the particular crop. Thus, $L = 0\ d^{-1}$.

Thus,

$$T_{L \rightarrow Ss} = L \tag{7-67}$$

where:

$T_{L \rightarrow Ss}$ = transfer factor from leaf to surface soil

Also,

$$T_{Lp \rightarrow Ss} = L \tag{7-68}$$

where:

$T_{L\text{-}Ss}$ = transfer factor from leaf surface (particulate matter) to surface soil

Note that the transfer of chemical from litter to surface water is not implemented in TRIM.FaTE at this time.

7.2.1.8 Senescence

Senesence is not considered in the current prototype of TRIM.FaTE. Senescence is the aging of plants, a process which affects the uptake of chemicals, growth, and plant parameters such as water content. If a user of TRIM.FaTE wants to include the process of senescence, candidate algorithms for changes in plant biomass may be found in Whicker and Kirchner (1987). Senescence is assumed to be negligible prior to August 1 through most of the United States.

7.2.1.9 Other Seasonal Issues

Plants only take up chemicals during the growing season, *i.e.*, the dates in the spring, summer, and fall between last frost and first frost. Although there may be uptake by conifers outside of the growing season, it is probably negligible for much of the non-growing season in cold environments (*e.g.*, in the Maine case study)" (Lindberg 1999b) and is not considered in TRIM.FaTE modeling purposes. To limit plant uptake only to the growing season, the user must specify the time period considered outside of the growing season.

An additional seasonal issue is deposition to the leaf surface compartment type. Tree foliage and grasses only intercept deposition when they are present. TRIM.FaTE assumes that there is no plant foliage present in the non-growing season, except for conifers. All deposition in deciduous forests, old fields, and agricultural systems in the non-growing season goes directly to

soil. Deposition to conifer foliage may continue in the winter, though accumulation of contaminants from particles or wet deposition is assumed to be negligible.

Chemical transformation within the plant is also assumed to cease in the non-growing season. There is no evidence to support or refute this assumption for most contaminants.

During the non-growing season, herbivores do not eat plants or make up this portion of their diet in any way. For herbivorous or omnivorous animals that do not hibernate or engage in winter sleep, the accumulation of contaminants from alternative, non-plant dietary sources may be underestimated in TRIM.FaTE.

7.2.2 SOIL DETRITIVORES

7.2.2.1 Earthworms

The uptake of chemicals by earthworms in TRIM.FaTE is described by an equation in the form of a time to equilibrium between the earthworms and soil. For simplicity, uptake is described as proportional to the concentration of the chemical in soil even though some studies suggest that a log-log regression between soil and earthworm concentrations is a more precise model of uptake.

$$C_{worm\text{-}dry} = K_{worm\text{-}Sr\text{-}dry} \times C_{Sr\text{-}dry} \quad (7\text{-}69)$$

where:

$C_{worm\text{-}dry}$	=	concentration of Hg in earthworm, kg/kg dry weight
$C_{Sr\text{-}dry}$	=	concentration of Hg in root-zone soil, kg/kg dry weight
$K_{worm\text{-}Sr\text{-}dry}$	=	earthworm-soil partition coefficient

If masses are converted to wet mass, then:

$$C_{worm} = (1\text{-}W_{worm}) \times C_{worm\text{-}dry} \quad (7\text{-}70)$$

where:

W_{worm}	=	water content of worm (kg water/kg worm)

and

$$C_{Sr} = (1\text{-}W_{Sr}) \times C_{Sr\text{-}dry} \quad (7\text{-}71)$$

where:

W_{Sr}	=	water content of soil (kg water/kg root zone soil)

Thus,

$$(1-W_{worm})\times C_{worm-dry} = \frac{(1-W_{worm})\times K_{worm-Sr-dry}}{1-W_{Sr}} \times (1-W_{Sr})\times C_{Sr-dry} \quad (7\text{-}72)$$

and

$$C_{worm} = K_{worm-Sr} \times C_{Sr} \quad (7\text{-}73)$$

where:

$K_{worm\text{-}Sr}$ = earthworm-soil partition coefficient (wet kg/kg per wet kg/kg), calculated to be

$$K_{worm-Sr} = \frac{(1-W_{worm})\times K_{worm-Sr-dry}}{1-W_{Sr}} \quad (7\text{-}74)$$

Thus,

$$\frac{dC_{worm}}{dt} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times K_{worm-Sr} \times C_{Sr} - \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] C_{worm} \quad (7\text{-}75)$$

where:

$t_{0.95}$ = time required to reach 95 percent of the steady-state value when C_{SR} is approximately constant with time (d^{-1})

If the areal density of worms is approximately constant with time, then:

$$\frac{dN_{worm}}{dt} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times V_{worm} K_{worm-Sr} \times \frac{N_{Sr}}{V_{Sr}} - \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] N_{worm} \quad (7\text{-}76)$$

where:

N_{worm} = mass of chemical in earthworms (kg)
N_{Sr} = total mass of chemical in all phases of bulk root zone soil (kg)
V_{Sr} = total volume of root zone soil, which contains worms (m^3)

$$V_{worm} = \frac{\rho area_{worm} A_S}{\rho vol_{worm}} \quad (7\text{-}77)$$

where:

A_S = area of soil surface (m^2)
$\rho area_{worm}$ = areal density of earthworm community in root-zone soil (kg worm fresh wt/m^2)
ρvol_{worm} = wet density of earthworm (kg/m^3)

Thus,

$$T_{Sr \rightarrow worm} = \left[\frac{-\ln(1-0.95)}{t_{0.95}} \right] \times \frac{\rho area_{worm}}{\rho vol_{worm}} K_{worm-Sr} \frac{1}{d_{Sr}} \quad (7\text{-}78)$$

$$T_{worm \rightarrow Sr} = -\left[\frac{-\ln(1-0.95)}{t_{0.95}} \right] \quad (7\text{-}79)$$

where:

$T_{Sr \rightarrow worm}$ = transfer factor from root-zone soil to worm
$T_{worm \rightarrow Sr}$ = transfer factor from worm to root-zone soil
d_{Sr} = depth of root-zone soil (V_{Sr}/A_S)

7.2.2.2 Soil Arthropods

An equation for the uptake of chemicals by soil arthropods may be derived similarly to that for earthworms. Much of the available data relates the concentration of a chemical in the fresh (wet weight) arthropod to that in food. The food may be plant matter rather than soil, but for the purpose of TRIM.FaTE, the uptake factors are assumed to apply to soil.

$$C_{arth} = K_{arth-Sr} \times C_{Sr} \quad (7\text{-}80)$$

where:

$K_{arth\text{-}Sr}$ = arthropod-soil partition coefficient (wet kg/kg per wet kg/kg)

Thus,

$$\frac{dC_{worm}}{dt} = \left[\frac{-\ln(1-0.95)}{t_{0.95}} \right] \times K_{arth-Sr} \times C_{Sr} - \left[\frac{-\ln(1-0.95)}{t_{0.95}} \right] C_{arth} \quad (7\text{-}81)$$

where:

$t_{0.95}$ = time required to reach 95 percent of the steady-state value when C_{SR} is approximately constant with time (d^{-1})

Thus,

$$\frac{dC_{arth}}{dt} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times K_{arth-Sr} \times C_{Sr} - \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] C_{arth} \quad (7\text{-}82)$$

where:

$t_{0.95}$ = time required to reach 95 percent of the steady-state value when C_{Sr} is approximately constant with time (d^{-1})

If the areal density of arthropods is approximately constant with time, then:

$$\frac{dN_{arth}}{dt} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times \rho area_{arth} A_S K_{arth-Sr} \times \frac{N_{Sr}}{M_{Sr}} - \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] N_{arth} \quad (7\text{-}83)$$

where:

N_{arth} = mass of chemical in arthropods (kg)
N_{Sr} = total mass of chemical in all phases of bulk root zone soil (kg)
M_{Sr} = total mass of root zone soil, which contains arthropods (kg)
A_S = area of soil surface (m^2)
$\rho area_{arth}$ = areal density of arthropod community in root-zone soil (kg arthropod fresh wt/m^2)

Thus,

$$T_{Sr \rightarrow arth} = \left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \times \rho area_{arth} \times A_S \times \frac{K_{arth-Sr}}{M_{Sr}} \quad (7\text{-}84)$$

$$T_{arth \rightarrow Sr} = -\left[\frac{-\ln(1-0.95)}{t_{0.95}}\right] \quad (7\text{-}85)$$

where:

$T_{Sr \rightarrow arth}$ = transfer factor from root-zone soil to arthropod
$T_{arth \rightarrow Sr}$ = transfer factor from arthropod to root-zone soil

7.2.2.3 Flying Insects

Flying insects are the food of insectivores (*e.g.*, tree swallows). It may be assumed that the concentration of a chemical in these organisms is equivalent to the concentration in benthic invertebrates such as the mayfly (see Section 7.3.2).

7.2.3 TERRESTRIAL MAMMALS AND BIRDS

Terrestrial wildlife, including mammals and birds, may be exposed to chemicals through food, soil, and water ingestion, and through inhalation of chemicals in air. In addition, chemicals can be taken up dermally, but the rate of sorption to the skin surface is unknown, the rate of uptake into the organism is unknown, and the quantity absorbed by the body (generally less than 3 percent) is low; thus, dermal uptake is not included in TRIM.FaTE. Elimination of chemicals from body tissues may occur through metabolic transformation of the chemical or excretion of the parent compound through urine, feces, milk (female mammals only), eggs (female birds and reptiles only), and excretion to fur, hair, or feathers. To account for these multiple routes of exposure and elimination, the generalized model implemented for all terrestrial wildlife is presented below. In addition, the algorithm applies to semiaquatic populations, such as loons and racoons. If particular rate constants are determined to be insignificant relative to others for a particular implementation of TRIM.FaTE (*e.g.*, excretion via eggs compared to excretion in urine or feces), these may be set to zero. Similarly, if rate constants for excretion and chemical transformation are determined with respect to the mass of a contaminant that is taken up in the diet rather than mass that is assimilated, the dietary assimilation efficiencies may be ignored. However, the assimilation efficiencies for inhalation must always be greater than zero.

$$\frac{dC_{wl}}{dt} = [(I_w \times C_w \times A_w) + (I_{SS} \times C_{SS} \times A_{SS}) + p_P(I_D \times C_L \times A_P) + p_P(I_D \times C_{LP} \times A_P) + p_{worm}(I_D \times C_{worm} \times A_{worm}) + p_{arth}(I_D \times C_{arth} \times A_{arth}) + p_{wl}(I_D \times C_{wl} \times A_{wl}) + p_f(I_D \times C_f \times A_f) + p_{BI}(I_D \times C_{BI} \times A_{BI}) + (I_A \times C_A \times A_A)] - [C_{wl} \times (E_m + E_u + E_l + E_e + E_f)] \quad (7\text{-}86)$$

where:

C_{wl}	=	total, whole body, internal concentration in wildlife (kg [chemical]/kg [body weight])
I_w	=	water ingestion rate (m^3/kg body weight/d)
C_w	=	concentration of chemical in water ingested by animal (kg/m^3)
A_w	=	assimilation efficiency of chemical from water (unitless)
I_{SS}	=	surface soil ingestion rate (kg/kg body weight/d)
C_{SS}	=	concentration of chemical in surface soil (kg/kg)
A_{SS}	=	assimilation efficiency of chemical from surface soil (unitless)
p_P	=	proportion of plant matter in diet (unitless)
I_D	=	dietary ingestion rate (kg/kg body weight/d)
C_L	=	concentration of chemical in leaf component of diet (kg/kg)
A_P	=	assimilation efficiency of chemical from plant in diet (unitless)
C_{LP}	=	mass of chemical on leaf surface with respect to mass of leaf (kg/kg)
p_{worm}	=	proportion of earthworm in diet (unitless)
C_{worm}	=	concentration of chemical in earthworm component of diet (kg/kg)
A_{worm}	=	assimilation efficiency of chemical from earthworm in diet (unitless)
p_{arth}	=	proportion of insect in diet (unitless)

C_{arth}	=	concentration of chemical in insect component of diet (kg/kg)
A_{arth}	=	assimilation efficiency of chemical from insect in diet (unitless)
p_{wl}	=	proportion of other wildlife in diet (unitless)
A_{wl}	=	assimilation efficiency of chemical from other wildlife in diet (unitless)
p_f	=	proportion of fish in diet (unitless)
C_f	=	concentration of chemical in fish component of diet (kg/kg, use correct size range)
A_f	=	assimilation efficiency of chemical from fish in diet (unitless)
p_{BI}	=	proportion of benthic invertebrates or emergent flying insects in diet (unitless)
C_{BI}	=	concentration of chemical in benthic invertebrates or flying insect component of diet (kg/kg)
A_{BI}	=	assimilation efficiency of chemical from benthic invertebrates or emergent flying insects in diet (unitless)
I_A	=	inhalation rate (m^3/kg body weight/d)
C_A	=	concentration of chemical in air, including vapor phase and particles (mg/m^3)
A_A	=	assimilation efficiency of chemical from air (unitless)
E_m	=	chemical transformation (d^{-1})
E_u	=	chemical elimination through excretory processes (urine and feces)(d^{-1})
E_l	=	chemical elimination through lactation (milk production, mammals only) (d^{-1})
E_e	=	chemical elimination through egg production, birds only (d^{-1})
E_f	=	chemical elimination from fur, feathers or hair (d^{-1})

Because the source of drinking water is not usually known and may include puddles, the uptake of the chemical from water may be ignored for all species except the semiaquatic, which are associated with a single water body.

Thus, for a population,

$$\frac{dN_{wl}}{dt} = \rho area_{wl} \times A_S \times [\frac{I_w \times N_w \times A_w}{V_w} + \frac{I_{SS} \times N_{SS} \times A_{SS}}{V_{SS} \times \rho vol_{SS} wet} + \frac{p_P \times I_D \times N_L \times A_P}{A_S \times \rho area_L}$$
$$\frac{p_P \times I_D \times N_{LP} \times A_P}{A_S \times \rho area_L} + \frac{p_{worm} \times I_D \times N_{worm} \times A_{worm}}{A_S \times \rho area_{worm}} + \frac{p_{arth} \times I_D \times N_{arth} \times A_{arth}}{A_S \times \rho area_{arth}} \quad (7\text{-}87)$$
$$+ \frac{p_{wl} \times I_D \times N_{wl} \times A_{wl}}{A_S \times \rho area_{wl}} + \frac{p_f \times I_D \times N_f \times A_f}{A_{sw} \times \rho area_f} + \frac{p_{BI} \times I_D \times N_{BI} \times A_{BI}}{A_{sw} \times \rho area_{BI}} + \frac{I_A \times N_{AIR} \times A_A}{V_A}]$$
$$-[N_{wl} \times (E_m + E_u + E_l + E_e + E_f)]$$

where:

N_{wl}	=	mass of chemical in all wildlife species in parcel (kg)
$\rho area_{wl}$	=	wet wildlife biomass density per unit area (kg/m^3, may be calculated as number of animals times average body weight)

A_S	=	area of surface soil (m^2)
I_w	=	water ingestion rate (m^3/kg body weight/d)
N_w	=	mass of chemical in water source (kg)
V_w	=	volume of water (m^3)
A_w	=	assimilation efficiency of chemical from water (unitless)
I_{SS}	=	surface soil ingestion rate (kg/kg body weight/d)
N_{SS}	=	mass of chemical in surface soil (kg)
V_{SS}	=	volume of surface soil (kg)
$\rho vol_{SS}wet$	=	wet bulk density of soil (kg/m^3)
A_{SS}	=	assimilation efficiency of chemical from surface soil (unitless)
p_P	=	proportion of plant matter in diet (unitless)
I_D	=	dietary ingestion rate (kg/kg body weight/d)
N_L	=	mass of chemical in plant leaves (kg)
A_P	=	assimilation efficiency of chemical from plant in diet (unitless)
$\rho area_L$	=	areal biomass density of foliage (kg/m^2, wet weight)
N_{LP}	=	mass of chemical on surface of all foliage (kg)
p_{worm}	=	proportion of earthworm in diet (unitless)
N_{worm}	=	mass of chemical in earthworms (kg)
A_{worm}	=	assimilation efficiency of chemical from earthworm in diet (unitless)
$\rho area_{worm}$	=	areal biomass density of earthworms (kg/m^2, wet weight)
p_{arth}	=	proportion of soil arthropods in diet (unitless)
N_{arth}	=	mass of chemical in soil arthropods (kg)
A_{arth}	=	assimilation efficiency of chemical from soil arthropods in diet (unitless)
p_{wl}	=	proportion of terrestrial wildlife in diet (unitless)
N_{wl}	=	mass of chemical in wildlife component of diet (kg)
A_{wl}	=	assimilation efficiency of chemical from other wildlife in diet (unitless)
p_f	=	proportion of fish in diet (unitless)
N_f	=	mass of chemical in fish (kg, use correct size range for diet)
A_f	=	assimilation efficiency of chemical from fish in diet (unitless)
$\rho area_f$	=	areal biomass density of fish (kg/m^2, wet weight, use correct size range for diet)
$\rho area_{arth}$	=	areal biomass density of insect (kg/m^2)
p_{BI}	=	proportion of benthic invertebrates or emergent flying insects in diet (unitless)
N_{BI}	=	mass of chemical in benthic invertebrates or emergent flying insects (kg)
A_{BI}	=	assimilation efficiency of chemical from benthic invertebrates or flying insects in diet (unitless)
A_{sw}	=	area of surface of surface water body (m^2)
$\rho area_{bi}$	=	areal biomass density of benthic invertebrates (kg/m^2, wet weight)
I_A	=	inhalation rate (m^3/kg body weight/d)
N_{AIR}	=	mass of chemical in air, including vapor phase and particles (kg)
V_A	=	volume of air (m^3)

A_A = assimilation efficiency of chemical from air (unitless)
E_m = chemical transformation (d^{-1})
E_u = chemical elimination through excretory processes (urine and feces) (d^{-1})
E_l = chemical elimination through lactation (milk production, mammals only) (d^{-1})
E_e = chemical elimination through egg production, birds only (d^{-1})
E_f = chemical elimination from fur, feathers or hair (d^{-1})

The TRIM.FaTE model has been parameterized for many wildlife species. These are listed in Table 7-1. Species-specific parameters, including body weights; water, soil, and food ingestion rates; and inhalation rates are presented as means in Appendix A.

Table 7-1
Terrestrial and Semiaquatic Vertebrate Compartment Types Defined for TRIM.FaTE

Compartment Type (Trophic Functional Group)	Representative Subgroup or Species
Terrestrial Omnivore	White-footed Mouse
Semi-aquatic Piscivore	Bald Eagle Common Loon Mink Belted Kingfisher
Terrestrial Insectivore	Black-capped Chickadee
Semi-aquatic Herbivore	Mallard
Terrestrial Predator/Scavenger	Red-tailed Hawk Long-tailed Weasel
Semi-aquatic Insectivore	Tree Swallow
Terrestrial Vertebrate Herbivore	White-tailed Deer Mule Deer Black-tailed Deer Meadow Vole Long-tailed Vole
Semi-aquatic Omnivore	Raccoon
Terrestrial Ground-invertebrate Feeder	Short-tailed Shrew Trowbridge Shrew

It is advisable for the user to turn on and off wildlife algorithms, to reflect:

- Winter sleep or hibernation;
- Migration;
- Timing of egg laying; and
- Timing of lactation.

These seasonal components of TRIM.FaTE have not yet been implemented.

7.3 ALGORITHMS FOR AQUATIC BIOTA

Aquatic compartment types in TRIM.FaTE are listed in Table 7-2.

Table 7-2
Aquatic Compartment Types in the TRIM.FaTE Prototype

Compartment Type (Trophic Functional Group)	Representative Subgroup or Species
Algae	Generalized Algal Species
Macrophyte	*Elodea densa*
Water Column Herbivore	Bluegill
Water Column Omnivore	Channel Catfish
Water Column Carnivore	Largemouth Bass
Benthic Invertebrate (Herbivore)	Mayfly
Benthic Omnivore	Channel Catfish
Benthic Carnivore	Largemouth Bass

7.3.1 AQUATIC PLANTS

Aquatic vegetation is included as two separate compartment types, algae and macrophytes. Water is assumed to be the primary chemical source for both groups and is the only pathway included in TRIM.FaTE. The algal compartment type is considered to be comprised primarily of phytoplankton, for which water is clearly the primary chemical source. Although rooted macrophytes derive some nutrients and chemicals from the sediment source, direct uptake from water is the primary pathway (Ribeyre and Boudou 1994).

7.3.1.1 Algae

At present, the only available algorithm for the uptake of contaminants by algae is specific to mercury. It is presented in Section A.1.2 of Appendix A.

7.3.1.2 Macrophytes

Uptake by aquatic macrophytes is given by the following concentration-based equation for the chemical flux rate.

$$F_{mp} = k_{mp,acc-sw} V_{mp} C_{sw} - k_{mp,dep-sw} V_{mp} C_{mp} \quad (7\text{-}88)$$

where:

F_{mp}	=	net flux of chemical in the macrophyte, (µg/day)
$k_{mp,acc\text{-}sw}$	=	bioaccumulation rate constant for surface water (day^{-1})
V_{mp}	=	volume of the macrophyte (L)
C_{sw}	=	chemical concentration in water (µg/L)
$k_{mp,dep\text{-}sw}$	=	depuration rate constant for surface water (day^{-1})
C_{mp}	=	chemical concentration in macrophyte (µg/L).

The rate constants $k_{mp,acc\text{-}sw}$ and $k_{mp,dep\text{-}sw}$, for nonionic organic chemicals are estimated using the following equations:

$$1/k_{mp,acc-sw} = 0.0020 + 500/K_{ow} \tag{7-89}$$

$$1/k_{mp,dep-sw} = 1.58 + 0.000015\ K_{ow} \tag{7-90}$$

The rate constants $k_{mp,acc\text{-}sw}$ and $k_{mp,dep\text{-}sw}$ for chemicals other than nonionic organic pollutants were derived from bioconcentration factors using the time-to-steady-state conversion as follows:

$$k_{mp,acc-sw} = \left[\frac{-\ln(1-\alpha)}{t_\alpha}\right] \times K_{w-mp} \tag{7-91}$$

$$k_{mp,dep-sw} = \left[\frac{-\ln(1-\alpha)}{t_\alpha}\right] \tag{7-92}$$

where:

$K_{w\text{-}mp}$	=	water-macrophyte partition coefficient
t_α	=	time required to reach 100α percent of the steady-state value when the concentration in water is approximately constant with time
α	=	fraction of steady-state attained

The transfer of chemical mass from water to the macrophyte is given by:

$$\frac{dN_{mp}}{dt} = k_{mp,acc-sw}\ V_{mp}\ \frac{N_w}{V_w} - k_{mp,dep-sw}\ N_{mp} \tag{7-93}$$

where:

N_{mp}	=	mass of chemical in the macrophyte (ug)
$k_{mp,acc\text{-}sw}$	=	bioaccumulation rate constant for surface water (day^{-1})
V_{mp}	=	volume of the macrophyte (L)

N_w = mass of chemical in water (ug)
V_w = volume of water in the cell (L)
$k_{mp,dep\text{-}sw}$ = depuration rate constant for surface water (day^{-1})

The transfer factors for water to macrophytes and for macrophytes to water are given by:

$$T_{w \rightarrow mp} = \frac{V_{mp}\, k_{mp,acc-sw}}{V_w} \tag{7-94}$$

$$T_{bi \rightarrow mp} = k_{mp,dep-sw} \tag{7-95}$$

7.3.2 BENTHIC INFAUNA

The benthic community is typically comprised of many different classes and species of organisms, including those from the phyla Mollusca (*e.g.*, clams and snails), Annelida (oligochaetes), and Arthropoda (*e.g.*, insects and crustaceans). All trophic levels are represented within this community. This is true even within some families of insects, such as the mayflies and chironomids. Although all trophic transfers within the benthic community could be modeled, that is beyond the scope and needs of TRIM.FaTE. Rather, all benthic infauna are considered to represent the lowest heterotrophic level of the benthic food chain. The current model construct identifies this group as the "Benthic Herbivores."

An explicit dietary uptake component is not practical, given the highly variable diet among benthic infauna. Rather, uptake is modeled based on the extraction of chemical from water (interstitial or overlying) or sediment. It should be noted that at this time only one chemical source (water or sediment) is considered. Selection of the primary source of contamination is chemical dependent. Neutral organic chemicals (*e.g.*, PAHs) are typically evaluated based on uptake from water. If interstitial water is used the results often are considered representative of total sediment exposures. Uptake of metals (*i.e.*, mercury) is based on uptake data from bulk sediments. Sediment chemical concentrations are not apportioned to separate inorganic and organic (living and detrital matter) compartments in TRIM.FaTE. Thus uptake from sediment implicitly includes transfers from algal and detrital matter to the "Benthic Herbivores."

Immature burrowing mayflies (*Hexagenia spp.*) are used as the representative benthic invertebrates for both water and sediment exposures. They are common throughout the United States, represent an important fish forage resource, and are relatively well studied by aquatic ecologists and toxicologists.

7.3.2.1 Water to Benthic Infauna Transfers

Uptake from water is given by the following equation:

$$\frac{dC_{bi}}{dt} = k_{bi,acc-w}\, C_w - k_{bi,dep-w}\, C_{bi} \tag{7-96}$$

where:

C_{bi} = benthic invertebrate concentration (µg/g)
C_w = water (interstitial or overlying) concentration (µg/L)
$k_{bi,acc-w}$ = uptake rate constant for water (day^{-1})
$k_{bi,dep-w}$ = depuration rate constant for water.

The rate constants $k_{bi,acc-w}$ and $k_{bi,dep-w}$ may be derived from the bioconcentration factors using the time-to-steady-state conversion.

$$k_{bi,acc-w} = \left[\frac{-\ln(1-\alpha)}{t_\alpha}\right] \times K_{w-bi} \tag{7-97}$$

$$k_{bi,dep-w} = \left[\frac{-\ln(1-\alpha)}{t_\alpha}\right] \tag{7-98}$$

where:

K_{w-bi} = water-benthic infauna partition coefficient.

Converting to mass units (N) yields the following equation:

$$\frac{dN_{bi}}{dt} = n_{bi}\, m_{bi}\, k_{bi,acc-w}\, \frac{N_w}{V_w} - k_{bi,dep-w}\, N_{bi} \tag{7-99}$$

where:

N_{bi} = mass of chemical in organisms comprising the benthic invertebrate compartment type (µg)
n_{bi} = number of organisms comprising the benthic invertebrate compartment type
m_{bi} = mass of individual organisms comprising the benthic invertebrate compartment type
N_w = mass of chemical in water (µg)
V_w = volume of water in the cell (L)

Thus the transfer factors for water (interstitial or overlying) to benthic invertebrates and for benthic invertebrates to water are given by:

$$T_{w \rightarrow bi} = \frac{n_{bi}\, m_{bi}\, k_{bi,acc-w}}{V_w} \tag{7-100}$$

$$T_{bi \rightarrow w} = k_{bi,dep-w} \tag{7-101}$$

7.3.2.2 Sediment to Benthic Infauna Transfers

Uptake from sediment is given by the following equation:

$$\frac{dC_{bi}}{dt} = k_{bi,acc-sed}\, C_{sed} - k_{bi,dep-sed}\, C_{bi} \tag{7-102}$$

where:

C_{bi}	=	benthic invertebrate concentration (µg/g)
C_{sed}	=	Bulk sediment concentration (µg/g)
$k_{bi,acc-sed}$	=	uptake rate constant for sediment (day^{-1})
$k_{bi,dep-sed}$	=	depuration rate constant for sediment.

The rate constants $k_{bi,acc-sed}$ and $k_{bi,dep-sed}$ may be derived from bioconcentration factors using the time-to-steady-state conversion.

$$k_{bi,acc-sed} = \left[\frac{-\ln(1-\alpha)}{t_\alpha}\right] \times K_{sed-bi} \tag{7-103}$$

$$k_{bi,dep-sed} = \left[\frac{-\ln(1-\alpha)}{t_\alpha}\right] \tag{7-104}$$

where:

K_{sed-bi}	=	sediment-benthic invertebrate partition coefficient
t_α	=	time required to reach 100α percent of the steady-state value when the concentration in water is approximately constant with time
α	=	fraction of steady-state attained

Converting to mass units (N) yields the following equation:

$$\frac{dN_{bi}}{dt} = n_{bi}\, m_{bi}\, k_{bi,acc-sed} \frac{N_{sed}}{V_{sed}\, \rho_{sed}} - k_{bi,dep-sed}\, N_{bi} \tag{7-105}$$

where:

N_{bi}	=	mass of chemical in organisms comprising the benthic invertebrate compartment type (μg)
n_{bi}	=	number of organisms comprising the benthic invertebrate compartment type
m_{bi}	=	mass of individual benthic invertebrates
N_{sed}	=	mass of chemical in sediment (μg)
V_{sed}	=	volume of sediment in the cell (L)
ρ_{sed}	=	bulk density of sediment (g/L)

Thus the transfer factors for sediment to benthic invertebrates and for benthic invertebrates to sediment are given by:

$$T_{sed \rightarrow bi} = \frac{n_{bi}\, m_{bi}\, k_{bi,acc-sed}}{V_{sed}\, \rho_{sed}} \tag{7-106}$$

$$T_{bi \rightarrow sed} = k_{bi,dep-sed} \tag{7-107}$$

7.3.3 FISH

Fish represent five of the trophic compartment types originally included in TRIM.FaTE: the Benthic omnivore and carnivore and the water column herbivore, omnivore, and carnivore. Two alternative approaches are used to estimate chemical uptake by fish in TRIM.FaTE, a bioenergetic-based kinetic model and a time-to-steady-state-based kinetic model. Each type has strengths and weaknesses which make including both appropriate at this time. The bioenergetic-based model is ideal for explicitly incorporating multiple exposure pathways, but parameterization is more difficult, especially for elimination rates. Parameters for the time-to-steady-state-based kinetic model are generally available, but multiple pathways cannot be explicitly incorporated simultaneously and the time required to reach a "steady-state" may be uncertain for strongly bioaccumulated chemicals. Currently, the bioenergetic model is parameterized for PAHs and mercury, whereas the time-to-steady-state model is parameterized for mercury only.

The current structure of TRIM.FaTE has five trophic levels that are represented by fish. They are presented as two separate food chains, one for water column organisms and one for benthic organisms (see blue print). The water column food chain has no linkages to benthic organisms, implying that this is a pelagic food chain. However, most applications of TRIM.FaTE will be better represented by a littoral food chain, which includes linkages between the water column and benthic food chains. The blue print shows the benthic food chain linked to rooted macrophytes and benthic algae, but not to planktonic algae. Thus, neither food chain alone adequately represents a littoral food chain.

To overcome this with minimal modification of the model architecture, each food chain was assumed to be linear but individual species were assumed to reside in more than one food chain or trophic level. That is, water column carnivores consume 100 percent water column omnivores, water column omnivores consume 100 percent water column herbivores (planktivores), benthic carnivores consume 100 percent benthic omnivores, benthic omnivores consume 100 percent benthic invertebrates. However, a given piscivore (e.g., largemouth bass) may consume omnivores from both food chains (e.g., 50 percent water column omnivores and 50 percent benthic omnivores). This is accounted for in the mass transfer formulas by dividing the total biomass of the given piscivorous species into each food chain. In the largemouth bass example, 50 percent of the biomass is counted in each food chain. The mass of fish in each trophic level is derived from studies of the biomass of individual species in various systems and studies of feeding strategies of those species.

7.3.3.1 Bioenergetic-based Kinetic Model

The following model for estimating pollutant concentrations in fish (Thomann 1989) was used as a starting point in the derivation of the transfer probabilities associated with the fish compartment type:

$$\frac{dC_F}{dt} = k_u \times C_{WD} + k_D \times \sum P_i \times C_{D,i} - (R_E + k_{eg} + k_E + k_G) \times C_F \qquad (7\text{-}108)$$

where:

C_F	=	concentration in fish (µg/kg)
k_u	=	uptake rate constant from water via the gills (1/kg-day)
C_{WD}	=	dissolved chemical concentration in water (µg/L)
k_D	=	chemical uptake from food (kg food/kg fish/day)
P_i	=	proportion of the diet consisting of food item I
$C_{D,i}$	=	chemical concentration in food item i (µg/kg)
k_{eg}	=	rate constant for elimination via the gills (1/day)
k_E	=	rate constant for elimination via fecal egestion (1/day)
R_E	=	rate constant for metabolic transformation of chemical (1/day)
k_G	=	rate constant for dilution of chemical concentration from growth (1/day).

For nonionic organic chemicals (PAHs), the chemical uptake rate constant k_u is estimated using the following formula:

$$k_u = 10^3 \left(\omega^{-\gamma} / p\right) E \qquad (7\text{-}109)$$

where:

k_u	=	chemical uptake rate constant (L/day-kg[w])
ω	=	body weight [g(wet)]
γ	=	allometric scaling factor (*e.g.*, 0.2 (Thomann 1989))

p = fraction lipid weight (kg[lipid]/kg[wet])
E = efficiency of transfer of chemical.

There is an apparent increase in assimilation efficiency for smaller organisms; therefore, organisms have been divided into two weight groups: less than 10 to 100 g (wet) and more than 100 g (wet) weight (Thomann 1989). The chemical assimilation efficiency (E) can be approximated for these two size classes of organisms as follows. For smaller organisms, the following equations should be used to estimate E:

For chemicals with log K_{ow} = 2-5, log E = -2.6 + 0.5 log K_{ow}
For chemicals with log K_{ow} = 5-6, log E = 0.8
For chemicals with log K_{ow} = 6-10, log E = 2.9 - 0.5 log K_{ow}

For larger organisms, the following equations should be used to estimate E:

For chemicals with log K_{ow} = 2-5, log E = -1.5 + 0.4 log K_{ow}
For chemicals with log K_{ow} = 5-6, log E = 0.5
For chemicals with log K_{ow} = 6-10, log E = 1.2 - 0.25 log K_{ow}

Thomann (1989) gives the excretion rate from gills using the following equation:

$$k_{eg} = \frac{k_u}{k_{ow}} \tag{7-110}$$

For mercury, the following simplifying assumptions apply: 1) a single elimination rate is used to describe elimination via the gills and egestion ($K_E = k_E + k_{eg}$), and 2) uptake from water is excluded from the mercury transfer equation because it is negligible (Trudel and Rasmussen 1997).

The mercury elimination rate constant (K_E) is given by the following bioenergetic model (Trudel and Rasmussen 1997) :

$$\ln K_E = 0.066\,T - 0.20 \ln W + 0.73E - 6.56 \tag{7-111}$$

where:

T = temperature (°C)
W = weight of fish (g)
E = exposure duration; 0=acute (<90 days), 1=chronic (>90 days)

Only chronic exposures apply to TRIM.FaTE. Therefore, the elimination rate constant is reduced to:

$$\ln K_E = 0.066\,T - 0.20 \ln W - 5.83 \tag{7-112}$$

Trudel and Rasmussen (1997) based the elimination rate on the clearance of methymercury only, because greater than 95 percent of mercury in fish is methymercury and the elimination of methymercury is much slower than that of inorganic mercury (*i.e.*, the overall rate is dominated by the elimination of methymercury).

The bioenergetic-based kinetic model is generally used to estimate concentrations in individual fish of a species. Following is the derivation of the fish model for the entire fish population. Initially the model is derived for a population of two fish and then generalized for the case of *n* fish, where *n* is the fish population. Initially, it is assumed that there is no uptake through other food items, and the elimination via fecal egestion and the metabolic transformation factors were neglected as they were considered second-order rates. Thus, for two fish with concentrations C_{f1}, and C_{f2}, the previous equation can be rewritten as:

$$\frac{dC_{f1}}{dt} = k_{u1} \times C_{WD} - k_{eg1} \times C_{f1} \tag{7-113}$$

$$\frac{dC_{f2}}{dt} = k_{u2} \times C_{WD} - k_{eg2} \times C_{f2} \tag{7-114}$$

To convert the concentrations to masses, it is assumed that:

$$C_{WD} = \frac{N_W}{V_W}, \tag{7-115}$$

$$C_{f1} = \frac{N_1}{m_1}, \tag{7-116}$$

$$C_{f2} = \frac{N_2}{m_2}, \tag{7-117}$$

where:

m_1	=	mass of fish 1 (kg)
m_2	=	mass of fish 2 (kg)
N_1	=	mass of chemical in fish 1 (µg)
N_2	=	mass of chemical in fish 2 (µg)
N_w	=	mass of chemical in surface water cell (µg)
V_w	=	volume of surface water cell (L).

Substituting yields:

$$\frac{d(N_1/m_1)}{dt} = k_{u1}\frac{N_W}{V_W} - k_{eg1}\frac{N_1}{m_1} \tag{7-118}$$

Adding these equations yields the mass transfer equations for the total fish compartment type, as follows:

$$\frac{d(N_2/m_2)}{dt} = k_{u2}\frac{N_W}{V_W} - k_{eg2}\frac{N_2}{m_2} \tag{7-119}$$

Making the simplifying assumptions that individual fish mass is represented by a population average m_f ($m_1 = m_2 = m_f$), and that $ku_1 = ku_2 = k_u$ and $k_{eg1} = k_{eg2} = k_{eg}$, yields:

$$\frac{d(N_1/m_1 + N_2/m_2)}{dt} = (k_{u1} + k_{u2})\frac{N_w}{V_w} - \left(k_{eg1}\frac{N_1}{m_1} + k_{eg2}\frac{N_2}{m_2} \right) \tag{7-120}$$

This equation can be generalized from 2 to n_f fish, with N_f (= N_1+N_2) being the total mass in the fish compartment type to yield the following generalized CMT equation for a fish compartment type:

$$\frac{d\left(\frac{N_1 + N_2}{m_f}\right)}{dt} = 2\ k_u\ \frac{N_W}{V_W} - k_{eg}\frac{N_1 + N_2}{m_f} \tag{7-121}$$

Generalizing this equation to include feeding yields the following food chain mass transfer equations for the individual fish species.

$$\frac{dN_1}{dt} = n_f\ k_u\ m_f\ \frac{N_W}{V_W} - k_{eg}\ N_f \tag{7-122}$$

It is important to note that the equations in their present form exclude dermal uptake as a significant exposure route. The equations include gill uptake (bioconcentration) and food uptake (biomagnification) as the two principal exposure routes. Following are the food web equations:

Aquatic herbivore (f_h ≡ fish herbivores) (100 percent macrophyte diet):

$$\frac{dN_{fh}}{dt} = n_{fh}\ k_u\ m_{fh}\ \frac{N_W}{V_W} - k_{eg}\ N_{fh} + n_{fh}\ m_{fh}\ F_d\ E\ \frac{N_{mp}}{V_{mp}} \tag{7-123}$$

where:

F_d = feeding rate constant (kg[prey]/kg[predator]-day)
E = efficiency of transfer of chemical.

The feeding rate (F_D) is given by the following bioenergetic model presented in Gobas (1993).

$$F_D = 0.022 \times V_F^{0.85} \times e^{(0.06 \times T)} \tag{7-124}$$

where:

V_F = mass of the fish (kg)
T = temperature (°C)

Aquatic omnivore (f_o = fish omnivore):

$$\frac{dN_{fo}}{dt} = n_{fo} k_u m_{fo} \frac{N_W}{V_W} - k_{eg} N_{fo} + n_{fo} m_{fo} F_d E \left(\alpha_{mp} \frac{N_{mp}}{m_{mp}} + \alpha_h \frac{N_h}{m_h} + \alpha_{bi} \frac{N_{bi}}{m_{bi}} \right) \tag{7-125}$$

Aquatic carnivore (f_c = fish carnivore):

$$\frac{dN_{fc}}{dt} = n_{fc} k_u m_{fc} \frac{N_W}{V_W} - k_{eg} N_{fc} + n_{fc} m_{fc} F_d E \left(\alpha_o \frac{N_o}{m_o} + \alpha_h \frac{N_h}{m_h} + \alpha_{bi} \frac{N_{bi}}{m_{bi}} \right) \tag{7-126}$$

Implicit in the previous equation is the assumption that the mass of an individual fish is constant over the time of the simulation. It may be noted that the dilution due to growth factor (k_G) is not included in the equation because k_G is based on concentrations, while the mass transfer equations are in mass units.

The generalized transfer factors for dietary items to a specific fish domain (*i.e.*, benthic omnivore, benthic carnivore, water column herbivore, water column omnivore, or water column carnivore), are given by:

$$T_{diet \rightarrow receptor(fish)} = \frac{n_{receptor} m_{receptor}}{n_{diet} m_{diet}} \times F_d \times E \tag{7-127}$$

Water to a specific fish domain (*i.e.*, benthic omnivore, benthic carnivore, water column herbivore, water column omnivore, or water column carnivore), using the bioenergetic-based kinetic model for nonionic organic chemicals is given by:

$$T_{water \rightarrow fish} = \frac{n_f m_f k_u}{V_w} \tag{7-128}$$

A specific fish domain (*i.e.*, benthic omnivore, benthic carnivore, water column herbivore, water column omnivore, or water column carnivore) to water, using the bioenergetic-based kinetic model for nonionic organic chemicals is given by:

$$T_{fish \rightarrow water} = k_{eg} \tag{7-129}$$

A specific fish domain (*i.e.*, benthic omnivore, benthic carnivore, water column herbivore, water column omnivore, or water column carnivore) to the water domain, using the bioenergetic-based kinetic model for mercury is given by:

$$T_{receptor\,(fish) \rightarrow water} = K_E \tag{7-130}$$

7.3.3.2 Time-to-steady-state-based Kinetic Model

The time-to-steady-state model is based on the assumption that one pathway accounts for the vast majority of the chemical uptake. Thus, only one chemical source is explicitly considered. The model is of the general form:

$$\frac{dC_{receptor}}{dt} = \left[\frac{-\ln(1-\alpha)}{t_\alpha}\right] \times K_{receptor-source} \times C_{source} - \left[\frac{-\ln(1-\alpha)}{t_\alpha}\right] C_{receptor} \tag{7-131}$$

where:

$K_{receptor\text{-}source}$	=	receptor-source partition coefficient
$C_{receptor}$	=	concentration in receptor
C_{source}	=	concentration in source
t_α	=	time required to reach 100α percent of the steady-state value when the concentration in the source is approximately constant with time
α	=	fraction of steady-state attained

If the sole chemical source is water, then $K_{receptor\text{-}source}$ is a bioconcentration factor. Bioaccumulation factors (BAFs) implicitly include uptake from food and water, though water is the identified source. This presumes that the concentration in the food item is essentially constant relative to the concentration in the water. An alternative approach is the use of dietary concentrations as the primary source. Thus, empirically derived accumulation data are used to derive factors for each trophic transfer and uptake from water is implicitly, rather than explicitly, included. This alternative is used herein.

Following this approach requires the dietary sources be restricted to one other trophic group. Thus intratrophic group transfers and multitrophic group transfers are not explicitly included. These transfers are implicitly included to the extent that the empirical data used to derive the transfer factors are from systems possessing those transfers. Thus, the "fit" of the model results for any given case study will be partly dependent on how well the food chains at the sites used to derive the transfer factors match the food chains at the case study site (*e.g.*, length of the food chains, number of interconnections, degree of intratrophic group transfer, etc.).

Restriction of the dietary pathway was achieved within TRIM.FaTE by redefining the generic trophic compartment types to represent a straight food chain of three or four segments. As noted in Section 7.3.2, the benthic herbivore compartment type is represented by all benthic invertebrates and the sediment (or interstitial water) is the chemical source. The benthic omnivore compartment type in this approach is the next trophic level up from the benthic invertebrates and the benthic carnivore compartment type contains those fish that consume the benthic omnivores. This is in contrast to the bioenergetic model, which accounts for the fractions of the omnivore diet from plants and herbivores.

A similar approach is used to configure the water column food chain. Three trophic levels are explicitly identified in TRIM.FaTE: the water column herbivore, omnivore, and carnivore. These correspond to the first, second, and third heterotrophic levels of the food chain, respectively. Chemical transfer is unidirectional from lower to higher trophic levels. Thus omnivores are assumed to consume herbivores only, rather than herbivores and algae. It is important to note that zooplankton have been implicitly included in the transfers from algae to herbivores. That is, the biomass and chemical mass associated with zooplankton are not explicitly tracked in TRIM.FaTE, but the dietary transfers are based concentration ratios for planktivorous fish and algae. Some studies provide the intermediate transfer factors for algae to zooplankton, but that compartment type is not currently maintained within TRIM.FaTE.

For each trophic level transfer, the general concentration based equation is converted to the following mass transfer equation:

$$\frac{dN_{receptor}}{dt} = n_{receptor}\, m_{receptor} \times \left[\frac{-\ln(1-\alpha)}{t_\alpha}\right] \times K_{receptor-diet} \times \frac{N_{diet}}{n_{diet}\, m_{diet}} - \left[\frac{-\ln(1-\alpha)}{t_\alpha}\right] N_{receptor} \quad (7\text{-}132)$$

where:

$N_{receptor}$	=	mass of chemical in the receptor
$n_{receptor}$	=	number of receptors
$m_{receptor}$	=	mass of individual receptors
N_{diet}	=	mass of chemical in items comprising the potential diet
n_{diet}	=	number of contaminated items comprising the potential diet
m_{diet}	=	mass of individual items comprising the potential diet

For example, the mass transfer equation for water column herbivores is given as:

$$\frac{dN_{f,wco}}{dt} = n_{f,wco}\, m_{f,wco} \times \left[\frac{-\ln(1-\alpha)}{t_\alpha}\right] \times K_{f,wco-f,wch} \times \frac{N_{f,wch}}{n_{f,wch}\, m_{f,wch}} - \left[\frac{-\ln(1-\alpha)}{t_\alpha}\right] N_{f,wco} \quad (7\text{-}133)$$

where:

$K_{f,wco\text{-}f,wch}$	=	fish, water column omnivore - fish, water column herbivore partition
$N_{f,wco}$	=	mass of chemical in fish comprising the water column omnivore compartment type
$n_{f,wco}$	=	number of fish comprising the water column omnivore compartment type
$m_{f,wco}$	=	mass of individual in fish comprising the water column omnivore compartment type
$N_{f,wch}$	=	mass of chemical in fish comprising the water column herbivore compartment type
$n_{f,wch}$	=	number of fish comprising the water column herbivore compartment type
$m_{f,wch}$	=	mass of individual fish comprising the water column herbivore compartment type

For each trophic level transfer, the generalized transfer factors for dietary items to a specific fish domain (*i.e.*, benthic omnivore, benthic carnivore, water column herbivore, water column omnivore, or water column carnivore) and for a specific fish domain to dietary items are given by:

$$T_{diet \rightarrow receptor(fish)} = \frac{n_{receptor}\, m_{receptor}}{n_{diet}\, m_{diet}} \times \left[\frac{-\ln(1-\alpha)}{t_{\alpha}} \right] \times K_{receptor-diet} \qquad (7\text{-}134)$$

$$T_{receptor(fish) \rightarrow diet} = \left[\frac{-\ln(1-\alpha)}{t_{\alpha}} \right] \qquad (7\text{-}135)$$

7.3.3.3 Other EPA Models for Bioaccumulation by Fish

Aquatox is a general ecological risk model that estimates the fate and effects of chemical and physical stressors in aquatic ecosystems (U.S. EPA 1998c). The model has been developed by the Office of Pollution Prevention and Toxics (OPPT) and the Office of Water (OW). The Bioaccumulation and Aquatic System Simulator (BASS), developed by the National Exposure Research Laboratory (NERL) of the Office of Research and Development (ORD), also simulates exposure and effects on fish (U.S. EPA 1999c). Aquatox and BASS are designed to predict effects of chemical contaminants and environmental factors on fish populations, whereas TRIM.FaTE is designed to estimate the fate and transport of chemicals throughout aquatic and terrestrial environment, with an emphasis on a collection of identical, individual fish. This difference in purpose results in several differences in structure: (1) Aquatox and BASS include chemical toxicity data; TRIM.FaTE does not (although TRIM.Risk is designed to include such a database); (2) the toxicological data in Aquatox and BASS are used to predict mortality, which is used to modify the structures of the models (*e.g.*, age-class structure and predator-prey

interactions); (3) in Aquatox, decomposition of dead fish and contaminants are linked to the dissolved oxygen levels in water, which affect populations; and (4) growth estimation of fish is fundamental to the population dynamics component of BASS, and growth is not included in the current prototype of TRIM.FaTE.

BASS (U.S. EPA 1999c) and Aquatox (U.S. EPA 1998c) are bioenergetic models of a multiple trophic level aquatic ecosystem. Aquatox, like TRIM.FaTE, provides an explicit steady-state option, whereas BASS does not. Like TRIM.FaTE, Aquatox has a Monte Carlo component to permit probabilistic estimates of exposure or risk. The developers of BASS plan to include metabolism of organic compounds in future versions of the model, but, unlike TRIM.FaTE, these transformations are not a feature of the current version (U.S. EPA 1999c). Components of Aquatox or Bass could be integrated with TRIM.FaTE. The challenge would be to preserve mass balance and to provide adequate links to all TRIM.FaTE compartment types that are connected to surface water and/or fish.

7.4 REVISIONS IN BIOTIC ALGORITHMS

Changes in algorithms since the PAH test case are identified in Table 7-4. It should be noted that PAH-specific parameters for generic algorithms have not been obtained and presented in Appendix A unless the algorithm was used in the 1998 test case.

Table 7-4
Differences Between Algorithms Implemented in the PAH Test Case and New Generic Algorithms that Would be Applicable to PAHs

Process	Algorithm or Assumption Implemented in 1998 PAH Test Case	1999 Generic Algorithm or Assumption
Deposition of particles to plant leaf	Particles deposited to plant leaf; leaf surface and leaf not separate compartment types	Particles deposited to plant leaf; leaf surface and leaf separate compartment types
Particle washoff from plant	Particles washed off leaf at rate equal to deposition rate; 5 percent particulate mass to air and 95 percent to soil	Particles washed off plant at rate in McCune and Lauver (1986), Sect. 7.2.1.1 of this volume; 100 percent of particles to soil
Transfer from surface of leaf to leaf and back	Not implemented because these were part of a single compartment type	First order rate constant, Sect. 7.2.1.1
Mesophyll resistance	Not implemented	Implemented as a generic algorithm, though assumed to be negligible for PAHs
Uptake by root	Uptake from soil water (see below)	Uptake from whole soil
Uptake by stem	Xylem and stem (see below) treated as compartment types; all uptake from soil via root	Stem treated as a compartment type; exchange between stem and leaf, and stem and root
Uptake by earthworm	Uptake from soil water (see below)	Uptake from whole soil
Uptake by soil arthropods	Not included in model	Uptake from whole soil
Uptake by algae	Not included in model	Uptake from surface water
Uptake by fish	Bioenergetic model implemented	Bioenergetic model is one of 2 options (other is time to equilibrium with diet)

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